Inventor Search

KRISHNAN 09/970,971

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L15 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:790526 HCAPLUS
DOCUMENT NUMBER: 133:350465
TITLE: Preparation of oligonucleotides having A-DNA form and B-DNA form **conformational geometry** as substrates for RNase H and nuclease resistance
INVENTOR(S): **Manoharan, Muthiah; Mohan, Venkatraman**
PATENT ASSIGNEE(S): Isis Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 132 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000066609 | A1 | 20001109 | WO 2000-US11913 | 20000503 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 6369209 | B1 | 20020409 | US 1999-303586 | 19990503 |
| EP 1180113 | A1 | 20020220 | EP 2000-928716 | 20000503 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |

PRIORITY APPLN. INFO.: US 1999-303586 A 19990503
WO 2000-US11913 W 20000503

AB Modified oligonucleotides contg. both A-form **conformation** geometry and B-form **conformation** geometry nucleotides are disclosed. The B-form geometry allows the oligonucleotide to serve as substrates for RNase H when bound to a target nucleic acid strand. The A-form geometry imparts properties to the oligonucleotide that modulate binding affinity and nuclease resistance. By utilizing C2' endo sugars or O4' endo sugars, the B-form characteristics are imparted to a portion of the oligonucleotide. The A-form characteristics are imparted via use of either 2'-O-modified nucleotides that have 3' endo geometries or use of end caps having particular nuclease stability or by use of both of these in conjunction with each other.

IT **149957-14-2P**, ISIS 2503 **181287-30-9P**
**216008-72-9P**, ISIS 14896 **216008-74-1P**, ISIS 14898
**216008-75-2P**, ISIS 14890 **216008-76-3P**, ISIS 14897
**216008-77-4P**, ISIS 14899 **216008-78-5P**, ISIS 13920
**256435-05-9P** **256435-06-0P** **256435-07-1P**
**303197-32-2P** **303197-33-3P** **303197-34-4P**
**304030-10-2P** **304030-11-3P** **304030-13-5P**
**304030-14-6P** **304030-15-7P** **304030-16-8P**
**304030-17-9P** **304030-18-0P** **304030-19-1P**
**304030-20-4P** **304030-21-5P** **304030-22-6P**
**304030-23-7P** **304030-24-8P** **304030-26-0P**
**304030-27-1P** **304030-28-2P** **304030-29-3P**
**304030-30-6P** **304030-31-7P** **304030-32-8P**

**304030-33-9P 304030-34-0P 304030-35-1P**
**304030-36-2P 304030-37-3P 304030-38-4P**
**304030-39-5P 304030-40-8P 304030-41-9P**
**304486-97-3P 304705-19-9P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(prepn. of oligonucleotides having A-DNA form and B-DNA form **conformational geometry** as substrates for RNase H and nuclease resistance)

RN 149957-14-2 HCAPLUS
CN Guanosine, P-thiothymidylyl-(3'.fwdarw.5')-2'-deoxy-P-thiocytidylyl-(3'.fwdarw.5')-2'-deoxy-P-thiocytidylyl-(3'.fwdarw.5')-2'-deoxy-P-thioguanylyl-(3'.fwdarw.5')-P-thiothymidylyl-(3'.fwdarw.5')-2'-deoxy-P-thiocytidylyl-(3'.fwdarw.5')-2'-deoxy-P-thioadenylyl-(3'.fwdarw.5')-P-thiothymidylyl-(3'.fwdarw.5')-2'-deoxy-P-thiocytidylyl-(3'.fwdarw.5')-2'-deoxy-P-thioguanylyl-(3'.fwdarw.5')-2'-deoxy-P-thiocytidylyl-(3'.fwdarw.5')-P-thiothymidylyl-(3'.fwdarw.5')-2'-deoxy-P-thiocytidylyl-(3'.fwdarw.5')-2'-deoxy-P-thiocytidylyl-(3'.fwdarw.5')-P-thiothymidylyl-(3'.fwdarw.5')-2'-deoxy-P-thiocytidylyl-(3'.fwdarw.5')-2'-deoxy-P-thioadenylyl-(3'.fwdarw.5')-2'-deoxy-P-thioguanylyl-(3'.fwdarw.5')-2'-deoxy- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 181287-30-9 HCAPLUS
CN DNA, d(G-G-C-T-G-[2'-O-(6-aminohexyl)]rU-C-T-G-C-G) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 216008-72-9 HCAPLUS
CN DNA, d(m5rUm[methylene(methylimino)oxy]rCm-sp-C-sp-G-sp-T-sp-C-sp-A-sp-T-sp-C-sp-G-sp-C-sp-T-sp-C-sp-C-sp-T-sp-C-sp-A-sp-G-sp-rGm[methylene(methylimino)oxy]rGm) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 216008-74-1 HCAPLUS
CN DNA, d(m5rUm[methylene(methylimino)oxy]rCm-sp-rCm[methylene(methylimino)oxy]rGm-sp-T-sp-C-sp-A-sp-T-sp-C-sp-G-sp-C-sp-T-sp-C-sp-C-sp-T-sp-C-sp-rAm[methylene(methylimino)oxy]rGm-sp-rGm[methylene(methylimino)oxy]rGm) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 216008-75-2 HCAPLUS
CN RNA, d(m5Um[methylene(methylimino)oxy]Cm-sp-Cm[methylene(methylimino)oxy]Gm-sp-m5Um[methylene(methylimino)oxy]Cm-sp-dA-sp-dT-sp-dC-sp-dG-sp-dC-sp-dT-sp-dC-sp-dC-sp-m5Um[methylene(methylimino)oxy]Cm-sp-Am[methylene(methylimino)oxy]Gm-sp-Gm[methylene(methylimino)oxy]Gm) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 216008-76-3 HCAPLUS
CN DNA, d(m5rUm[methylene(methylimino)oxy]rCm-rCm[methylene(methylimino)oxy]rGm-sp-T-sp-C-sp-A-sp-T-sp-C-sp-G-sp-C-sp-T-sp-C-sp-C-sp-T-sp-C-sp-rAm[methylene(methylimino)oxy]rGm-rGm[methylene(methylimino)oxy]rGm) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 216008-77-4 HCAPLUS
CN RNA, d(m5Um[methylene(methylimino)oxy]Cm-Cm[methylene(methylimino)oxy]Gm-m5Um[methylene(methylimino)oxy]Cm-sp-dA-sp-dT-sp-dC-sp-dG-sp-dC-sp-dT-sp-dC-sp-dC-sp-m5Um[methylene(methylimino)oxy]Cm-

Am[methylene(methylimino)oxy]Gm-Gm[methylene(methylimino)oxy]Gm) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 216008-78-5 HCAPLUS
CN RNA, (P-thio)([2'-O-(2-methoxyethyl)]m5U-[2'-O-(2-methoxyethyl)]C-[2'-O-(2-methoxyethyl)]C-dG-dT-dC-dA-dT-dC-dG-dC-dT-[2'-O-(2-methoxyethyl)]C-[2'-O-(2-methoxyethyl)]C-[2'-O-(2-methoxyethyl)]m5U-[2'-O-(2-methoxyethyl)]C-[2'-O-(2-methoxyethyl)]A-[2'-O-(2-methoxyethyl)]G-[2'-O-(2-methoxyethyl)]G-[2'-O-(2-methoxyethyl)]G) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 256435-05-9 HCAPLUS
CN DNA, d(P-thio)(A-T-G-C-A-T-T-C-T-G-C-C-C-C-C-C-A-A-G-[3'-O-(2-methoxyethyl)]rG-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]rA) (9CI) (CA INDEX NAME)

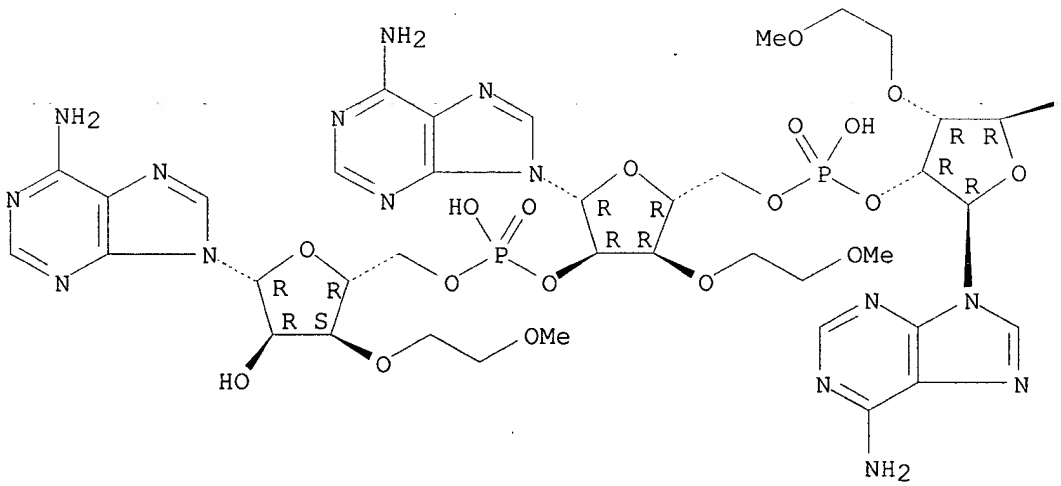
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 256435-06-0 HCAPLUS
CN DNA, d(A-sp-T-sp-G-sp-C-sp-A-sp-T-sp-T-sp-C-sp-T-sp-G-sp-C-sp-C-sp-C-sp-C-sp-C-sp-A-sp-A-sp-G-[3'-O-(2-methoxyethyl)]rG-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]rA) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 256435-07-1 HCAPLUS
CN DNA, d(P-thio)([3'-O-(2-methoxyethyl)]rA-(2'.fwdarw.5')-T-G-C-A-T-T-C-T-G-C-C-C-C-C-A-A-G-[3'-O-(2-methoxyethyl)]rG-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]rA) (9CI) (CA INDEX NAME)

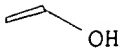
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 303197-32-2 HCAPLUS
CN Adenosine, 3'-O-(2-methoxyethyl)adenylyl-(2'.fwdarw.5')-3'-O-(2-methoxyethyl)adenylyl-(2'.fwdarw.5')-3'-O-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



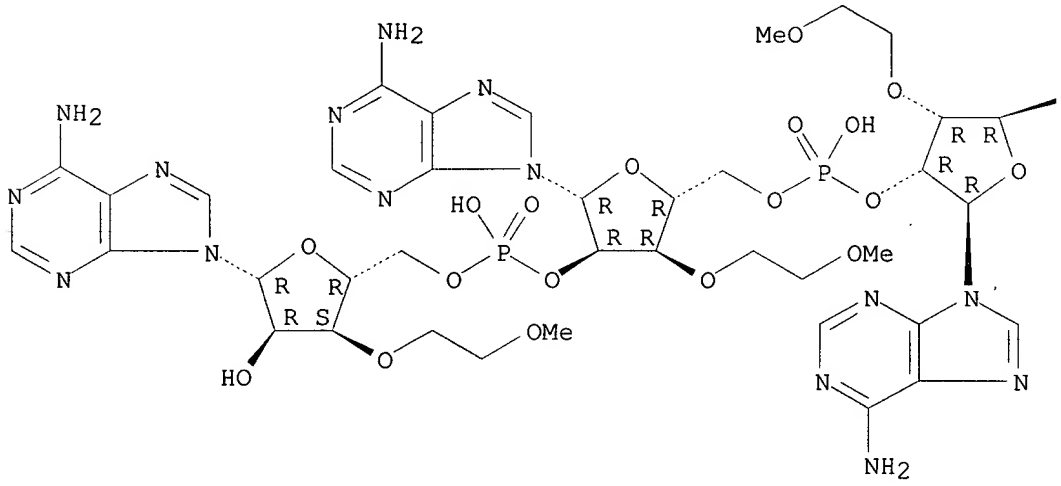
PAGE 1-B



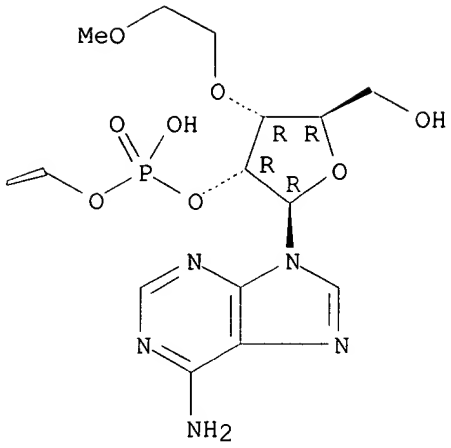
RN 303197-33-3 HCAPLUS
CN Adenosine, 3'-O-(2-methoxyethyl)adenylyl-(2'.fwdarw.5')-3'-O-(2-methoxyethyl)adenylyl-(2'.fwdarw.5')-3'-O-(2-methoxyethyl)adenylyl-(2'.fwdarw.5')-3'-O-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



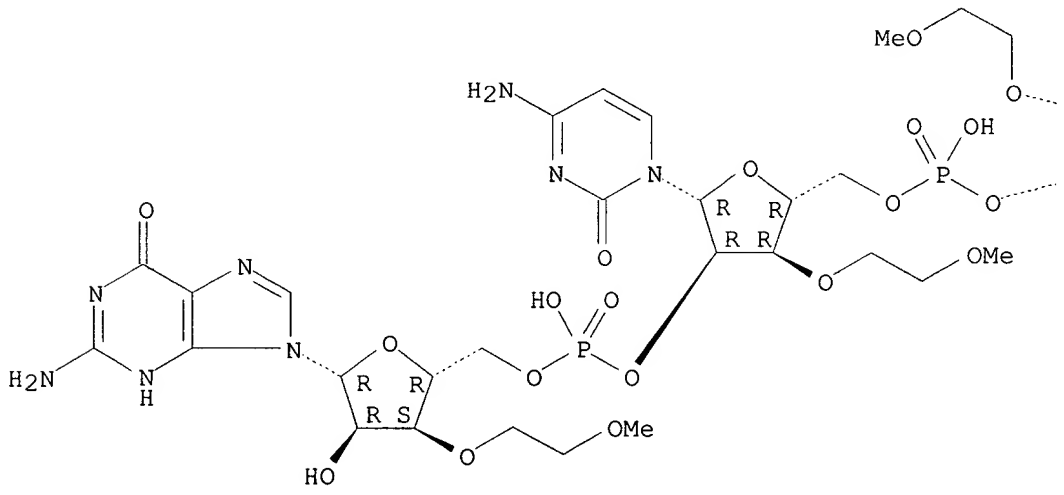
PAGE 1-B

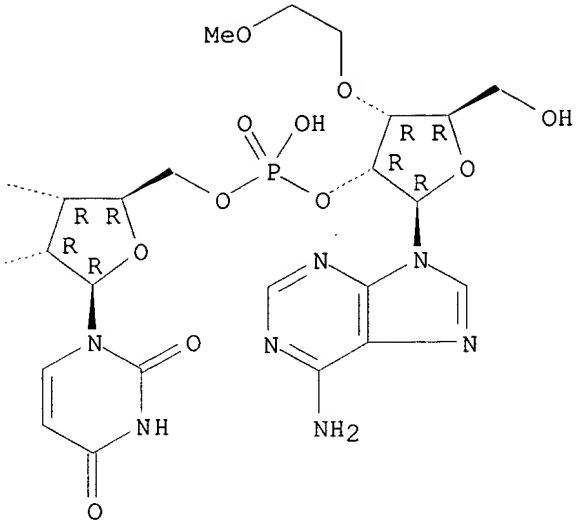


RN 303197-34-4 HCAPLUS
CN Guanosine, 3'-O-(2-methoxyethyl)adenylyl-(2'.fwdarw.5')-3'-O-(2-methoxyethyl)uridylyl-(2'.fwdarw.5')-3'-O-(2-methoxyethyl)cytidylyl-(2'.fwdarw.5')-3'-O-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





RN 304030-10-2 HCAPLUS
CN DNA, d(P-thio)(A-T-G-C-A-T-T-C-T-G-C-C-C-C-C-A-A-G-G-[3'-O-(2-methoxyethyl)]rA) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-11-3 HCAPLUS
CN DNA, d(P-thio)([3'-O-(2-methoxyethyl)]rA-(2'.fwdarw.5')-T-G-C-A-T-T-C-T-G-C-C-C-C-C-A-A-G-G-[3'-O-(2-methoxyethyl)]rA) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-13-5 HCAPLUS
CN DNA, d([3'-O-(2-methoxyethyl)]rA-(2'.fwdarw.5')-T-sp-G-sp-C-sp-A-sp-T-sp-T-sp-C-sp-T-sp-G-sp-C-sp-C-sp-C-sp-C-sp-C-sp-A-sp-A-sp-G-[3'-O-(2-methoxyethyl)]rG-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]rA) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-14-6 HCAPLUS
CN DNA, d(P-thio)([3'-O-(2-methoxyethyl)]rA-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-G-C-A-T-T-C-T-G-C-C-C-C-C-A-A-G-[3'-O-(2-methoxyethyl)]rG-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]rA) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-15-7 HCAPLUS
CN DNA, d([3'-O-(2-methoxyethyl)]rA-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-G-sp-C-sp-A-sp-T-sp-T-sp-C-sp-T-sp-G-sp-C-sp-C-sp-C-sp-C-sp-C-sp-A-sp-A-sp-G-[3'-O-(2-methoxyethyl)]rG-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]rA) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-16-8 HCAPLUS
CN RNA, [3'-O-(2-methoxyethyl)](2'.fwdarw.5')(C-G-C-G-A-A-m5rU-m5rU-C-G-C-G) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-17-9 HCAPLUS

CN DNA, d(T-C-C-T-T-G-G-G-G-G-C-A-G-A-A-T-G-C-A-T), complex with DNA d(P-thio)(A-T-G-C-A-T-T-C-T-G-C-C-C-C-C-A-A-G-G-[3'-O-(2-methoxyethyl)]rA) (1:1) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-18-0 HCAPLUS
CN DNA, d(T-C-C-T-T-G-G-G-G-G-C-A-G-A-A-T-G-C-A-T), complex with DNA d(P-thio)(A-T-G-C-A-T-T-C-T-G-C-C-C-C-C-A-A-G-[3'-O-(2-methoxyethyl)]rG-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]rA) (1:1) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-19-1 HCAPLUS
CN DNA, d(A-sp-T-sp-G-sp-C-sp-A-sp-T-sp-T-sp-C-sp-T-sp-G-sp-C-sp-C-sp-C-sp-C-sp-C-sp-A-sp-A-sp-G-[3'-O-(2-methoxyethyl)]rG-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]rA), complex with DNA d(T-C-C-T-T-G-G-G-G-G-C-A-G-A-A-T-G-C-A-T) (1:1) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-20-4 HCAPLUS
CN DNA, d(T-C-C-T-T-G-G-G-G-G-C-A-G-A-A-T-G-C-A-T), complex with DNA d(P-thio)([3'-O-(2-methoxyethyl)]rA-(2'.fwdarw.5')-T-G-C-A-T-T-C-T-G-C-C-C-C-C-A-A-G-G-[3'-O-(2-methoxyethyl)]rA) (1:1) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-21-5 HCAPLUS
CN DNA, d(T-C-C-T-T-G-G-G-G-G-C-A-G-A-A-T-G-C-A-T), complex with DNA d(P-thio)([3'-O-(2-methoxyethyl)]rA-(2'.fwdarw.5')-T-G-C-A-T-T-C-T-G-C-C-C-C-C-A-A-G-[3'-O-(2-methoxyethyl)]rG-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]rA) (1:1) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-22-6 HCAPLUS
CN DNA, d([3'-O-(2-methoxyethyl)]rA-(2'.fwdarw.5')-T-sp-G-sp-C-sp-A-sp-T-sp-T-sp-C-sp-T-sp-G-sp-C-sp-C-sp-C-sp-C-sp-C-sp-A-sp-A-sp-G-[3'-O-(2-methoxyethyl)]rG-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]rA), complex with DNA d(T-C-C-T-T-G-G-G-G-G-C-A-G-A-A-T-G-C-A-T) (1:1) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-23-7 HCAPLUS
CN DNA, d(T-C-C-T-T-G-G-G-G-G-C-A-G-A-A-T-G-C-A-T), complex with DNA d(P-thio)([3'-O-(2-methoxyethyl)]rA-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-G-C-A-T-T-C-T-G-C-C-C-C-C-A-A-G-[3'-O-(2-methoxyethyl)]rG-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]rA) (1:1) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-24-8 HCAPLUS
CN DNA, d([3'-O-(2-methoxyethyl)]rA-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-G-sp-C-sp-A-sp-T-sp-T-sp-C-sp-T-sp-G-sp-C-sp-C-sp-C-sp-C-sp-C-sp-A-sp-A-sp-G-[3'-O-(2-methoxyethyl)]rG-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]rA), complex with DNA d(T-C-C-T-T-G-G-G-G-G-C-A-G-A-A-T-G-C-A-T) (1:1) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-26-0 HCAPLUS
CN RNA, (Gm-Gm-Cm-m5Um-Gm-U-Cm5-m5Um-Gm-Cm-Gm) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-27-1 HCAPLUS

CN RNA, (Gm-Gm-Cm-m5Um-Gm-[2'-O-(6-aminohexyl)]U-Cm5-m5Um-Gm-Cm-Gm) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-28-2 HCAPLUS
CN DNA, d(G-G-C-T-G-[3'-O-(6-aminohexyl)]rU-(2'.fwdarw.5')-C-T-G-C-G) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-29-3 HCAPLUS
CN DNA, d(T-T-T-T-T-T-T-T-T-T-T-T-T-T-T-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-30-6 HCAPLUS
CN DNA, d(T-T-T-T-T-T-T-T-T-T-T-T-T-T-T-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]rU) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-31-7 HCAPLUS
CN DNA, d(P-thio)(T-T-T-T-T-T-T-T-T-T-T-T-T-T-T-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-32-8 HCAPLUS
CN DNA, d(P-thio)(T-T-T-T-T-T-T-T-T-T-T-T-T-T-T-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]rU) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-33-9 HCAPLUS
CN DNA, d(T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU-(2'.fwdarw.5')-[3'-O-(2-methoxyethyl)]m5rU) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-34-0 HCAPLUS
CN DNA, d(T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-sp-T-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]rU) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-35-1 HCAPLUS
CN DNA, d(P-thio)([3'-O-(3-aminopropyl)]rA-(2'.fwdarw.5')-T-G-m5rC-A-T-T-m5rC-T-G-m5rC-m5rC-m5rC-m5rC-m5rC-A-A-G-G-[3'-O-(3-aminopropyl)]rA) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-36-2 HCAPLUS
CN DNA, d(P-thio)([3'-O-(3-aminopropyl)]rA-(2'.fwdarw.5')-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]rG-[2'-O-(2-methoxyethyl)]m5rC-[2'-O-(2-methoxyethyl)]rA-T-T-m5C-T-G-m5C-m5C-m5C-m5C-m5C-[2'-O-(2-methoxyethyl)]rA-[2'-O-(2-methoxyethyl)]rA-[2'-O-(2-methoxyethyl)]rG-[2'-O-(2-methoxyethyl)]rG-[3'-O-(3-aminopropyl)]rA) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-37-3 HCAPLUS
CN DNA, d([3'-O-(3-aminopropyl)]rA-(2'.fwdarw.5')-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]rG-[2'-O-(2-methoxyethyl)]m5rC-[2'-O-(2-methoxyethyl)]rA-T-sp-T-sp-m5C-sp-T-sp-G-sp-m5C-sp-m5C-sp-m5C-sp-m5C-sp-m5C-sp-[2'-O-(2-methoxyethyl)]rA-[2'-O-(2-methoxyethyl)]rA-[2'-O-(2-methoxyethyl)]rG-[2'-O-(2-methoxyethyl)]rG-[3'-O-(3-aminopropyl)]rA) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-38-4 HCAPLUS
CN DNA, d([2'-O-(3-aminopropyl)]rA-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]rG-[2'-O-(2-methoxyethyl)]m5rC-[2'-O-(2-methoxyethyl)]rA-T-sp-T-sp-m5C-sp-T-sp-G-sp-m5C-sp-m5C-sp-m5C-sp-m5C-sp-m5C-sp-[2'-O-(2-methoxyethyl)]rA-[2'-O-(2-methoxyethyl)]rA-[2'-O-(2-methoxyethyl)]rG-[2'-O-(2-methoxyethyl)]rG-[2'-O-(3-aminopropyl)]rA) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-39-5 HCAPLUS
CN DNA, d(P-thio)([2'-O-(3-aminopropyl)]rA-[2'-O-(2-methoxyethyl)]m5rU-[2'-O-(2-methoxyethyl)]rG-[2'-O-(2-methoxyethyl)]m5rC-[2'-O-(2-methoxyethyl)]rA-T-T-m5C-T-G-m5C-m5C-m5C-m5C-m5C-[2'-O-(2-methoxyethyl)]rA-[2'-O-(2-methoxyethyl)]rA-[2'-O-(2-methoxyethyl)]rG-[2'-O-(2-methoxyethyl)]rG-[2'-O-(3-aminopropyl)]rA) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-40-8 HCAPLUS
CN DNA, d(P-thio)([2'-O-(3-aminopropyl)]rA-T-G-m5C-A-T-T-m5C-T-G-m5C-m5C-m5C-m5C-m5C-A-A-G-G-[2'-O-(3-aminopropyl)]rA) (9CI) (CA INDEX NAME)

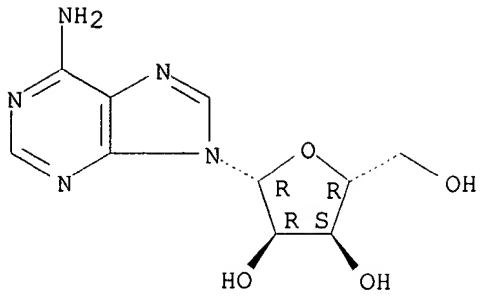
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304030-41-9 HCAPLUS
CN DNA, d(T-G-C-A-T-C-C-C-C-C-A-G-G-C-C-A-C-C-rAm[methylene(methylimino)oxy]m5rUm) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304486-97-3 HCAPLUS
CN DNA, d(m5rUm[methylene(methylimino)oxy]Gm-C-A-T-C-C-C-C-C-A-G-G-C-C-A-C-C-Am[methylene(methylimino)oxy]m5rUm) (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 304705-19-9 HCAPLUS
CN DNA, d(T-C-C-T-T-G-G-G-G-G-C-A-G-A-A-T-G-C-A-T), complex with DNA d(P-thio)(A-T-G-C-A-T-T-C-T-G-C-C-C-C-C-A-A-G-G-A) (1:1) (9CI) (CA INDEX NAME)

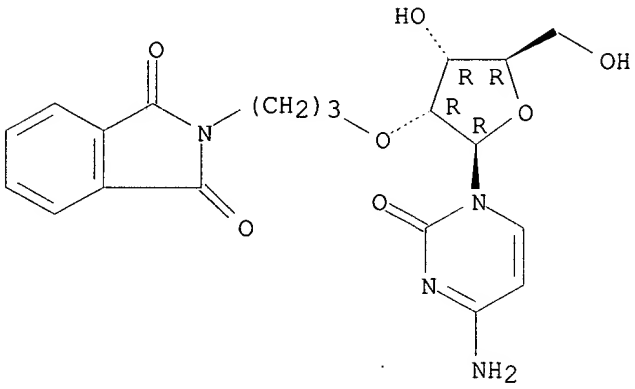
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT **58-61-7**, Adenosine, reactions **165381-50-0** **303197-31-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of oligonucleotides having A-DNA form and B-DNA form **conformational geometry** as substrates for RNase H and nuclease resistance)
RN 58-61-7 HCAPLUS
CN Adenosine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



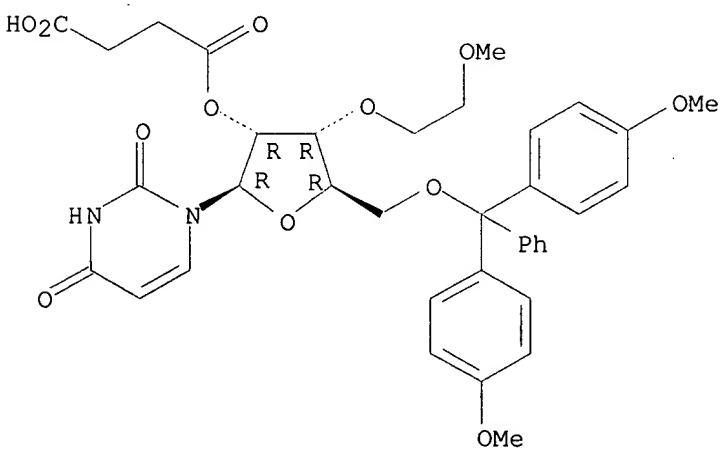
RN 165381-50-0 HCAPLUS
CN Cytidine, 2'-O-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 303197-31-1 HCAPLUS
CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-O-(2-methoxyethyl)-, 2'-(hydrogen butanedioate) (9CI) (CA INDEX NAME)

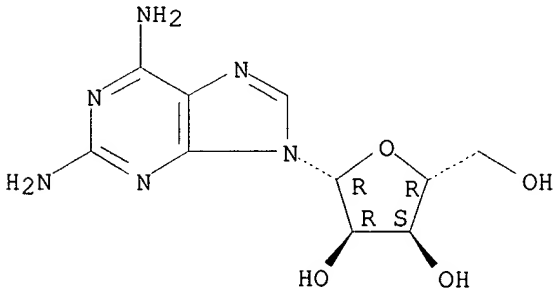
Absolute stereochemistry.



IT **2096-10-8P 136834-10-1P 156881-42-4P**
**156881-43-5P 156881-44-6P 156881-45-7P**
**163759-49-7P 165381-01-1P 165381-32-8P**
**165381-39-5P 165381-41-9P 165381-44-2P**
**165381-45-3P 168427-74-5P 170114-29-1P**
**256223-93-5P 256223-95-7P 256223-97-9P**
**256223-99-1P 256224-00-7P 256224-01-8P**
**256224-02-9P 256224-03-0P 256224-04-1P**
**256224-05-2P 256224-06-3P 256224-07-4DP,**
LCA-CPG support **256224-08-5DP**, LCA-CPG support
**256224-09-6DP**, LCA-CPG support **256224-10-9DP**, polymer
support **256224-11-0DP**, aminopropyl-CPG support
**256224-12-1P 256224-13-2P 256420-89-0P**
**303197-29-7P 303197-30-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of oligonucleotides having A-DNA form and B-DNA form **conformational geometry** as substrates for RNase H and nuclease resistance)

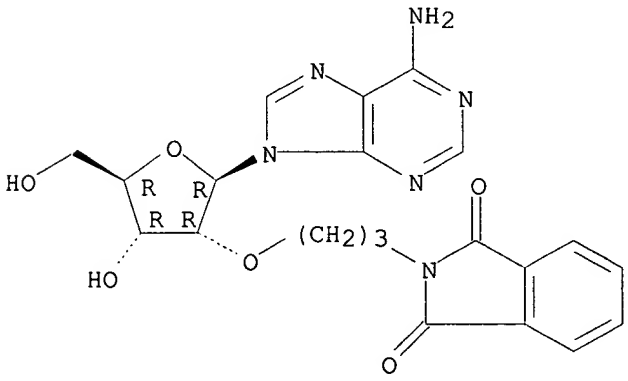
RN 2096-10-8 HCAPLUS
CN Adenosine, 2-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 136834-10-1 HCAPLUS
CN Adenosine, 2'-O-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]- (9CI) (CA INDEX NAME)

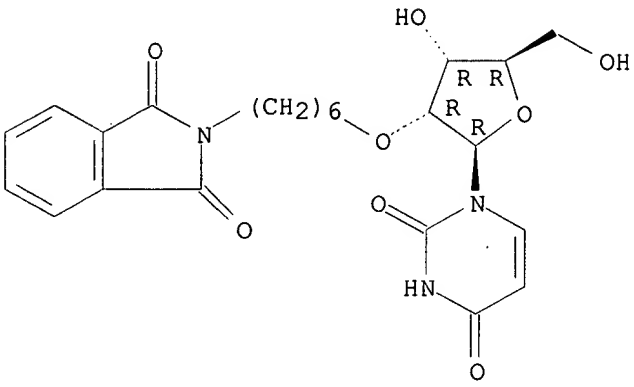
Absolute stereochemistry.



RN 156881-42-4 HCAPLUS

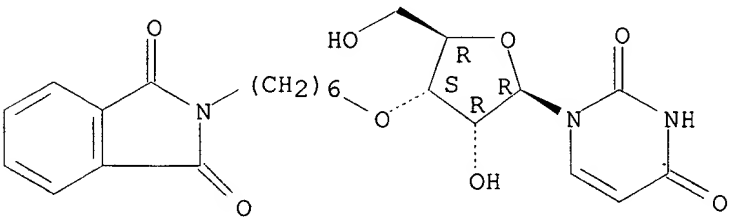
CN Uridine, 2'-O-[6-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)hexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



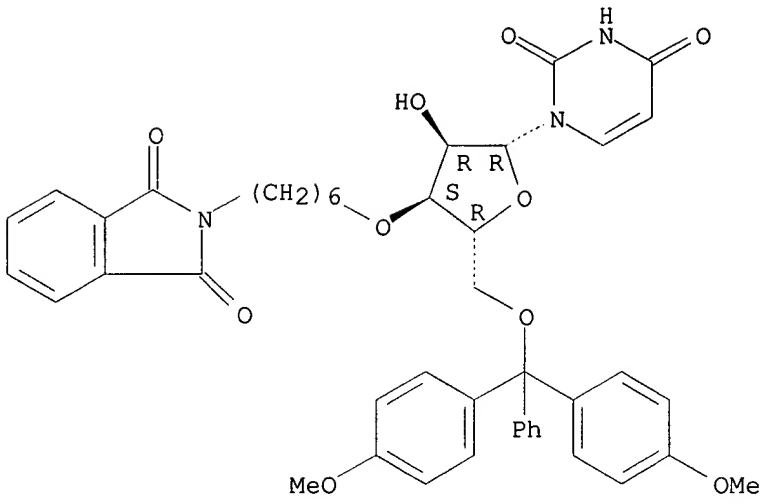
RN 156881-43-5 HCAPLUS
CN Uridine, 3'-O-[6-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)hexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



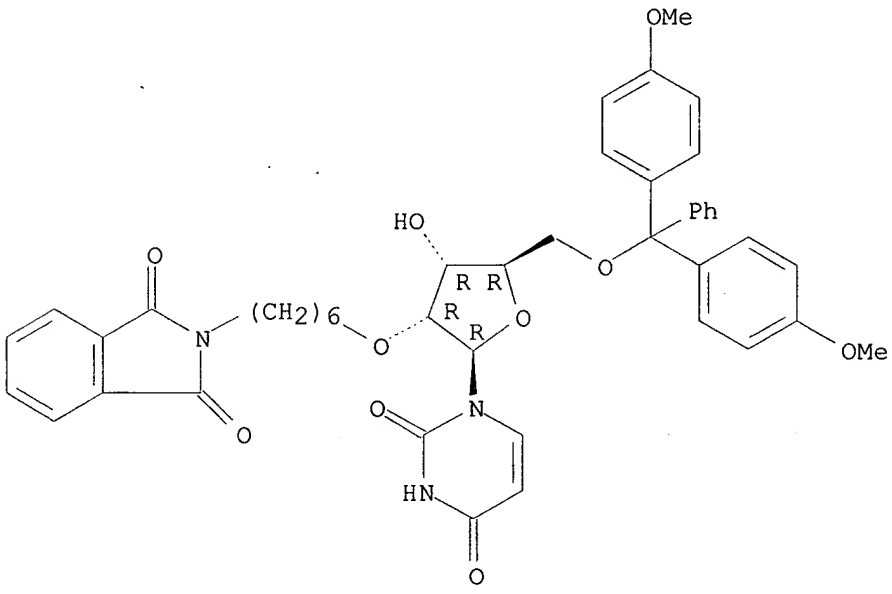
RN 156881-44-6 HCAPLUS
CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-O-[6-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)hexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



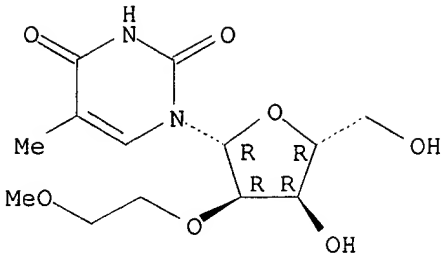
RN 156881-45-7 HCAPLUS
CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-O-[6-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)hexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



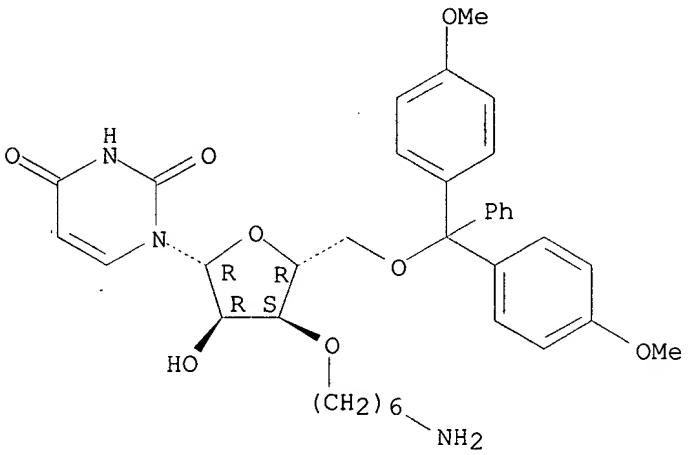
RN 163759-49-7 HCAPLUS
CN Uridine, 2'-O-(2-methoxyethyl)-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



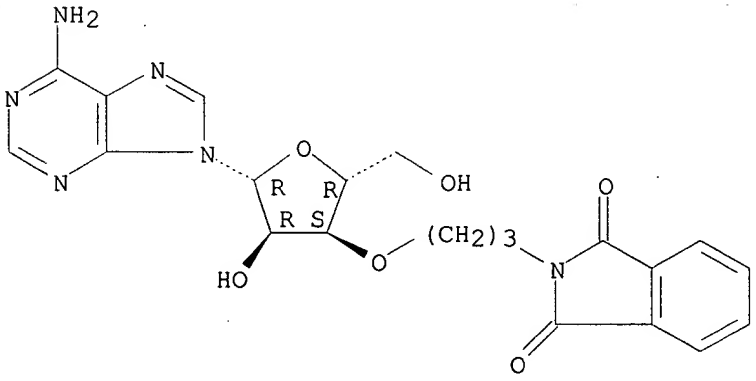
RN 165381-01-1 HCAPLUS
CN Uridine, 3'-O-(6-aminohexyl)-5'-O-[bis(4-methoxyphenyl)phenylmethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 165381-32-8 HCAPLUS
CN Adenosine, 3'-O-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]- (9CI) (CA INDEX NAME)

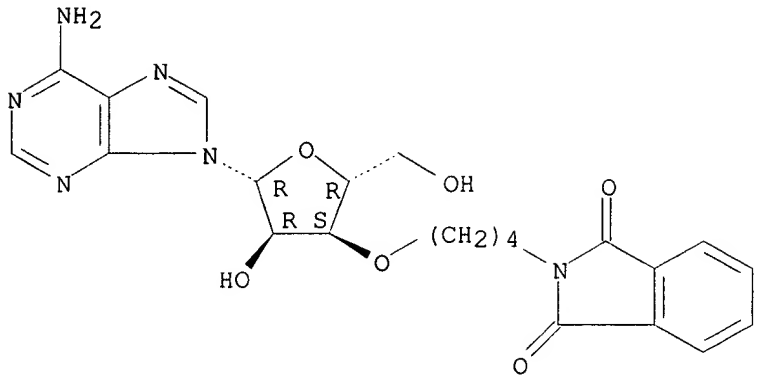
Absolute stereochemistry.



RN 165381-39-5 HCAPLUS
CN Adenosine, 3'-O-[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)butyl]- (9CI)

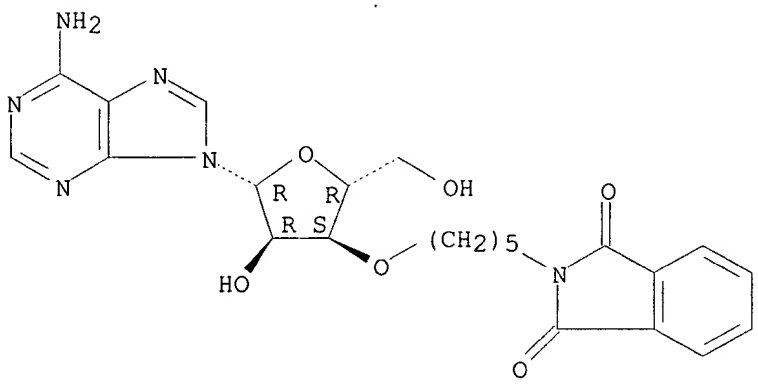
(CA INDEX NAME)

Absolute stereochemistry.



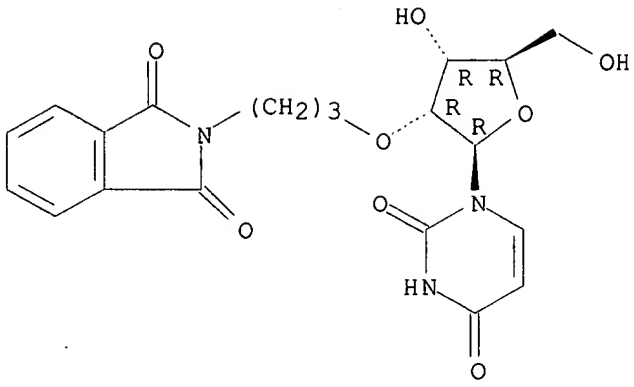
RN 165381-41-9 HCAPLUS
CN Adenosine, 3'-O-[5-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)pentyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



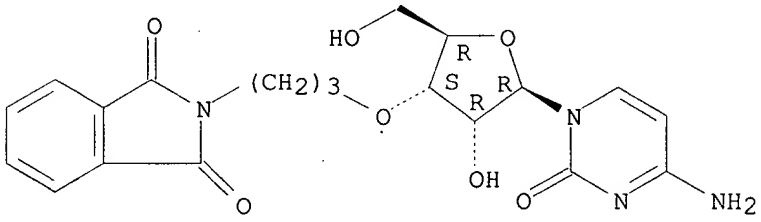
RN 165381-44-2 HCAPLUS
CN Uridine, 2'-O-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



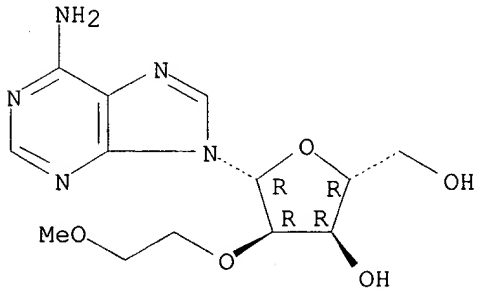
RN 165381-45-3 HCAPLUS
CN Cytidine, 3'-O-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



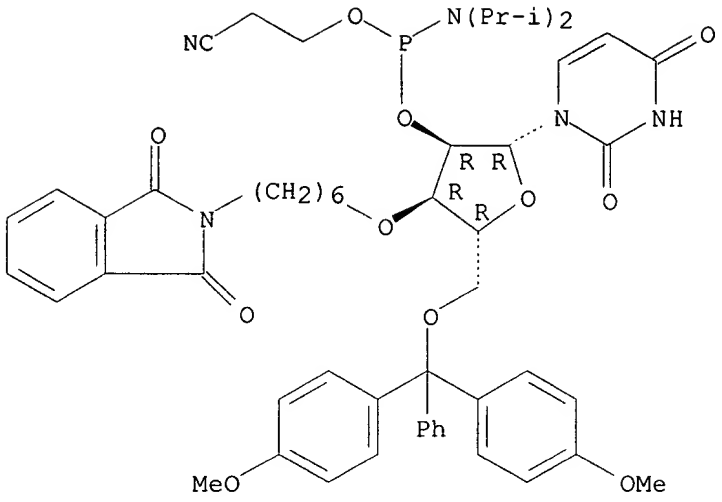
RN 168427-74-5 HCAPLUS
CN Adenosine, 2'-O-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



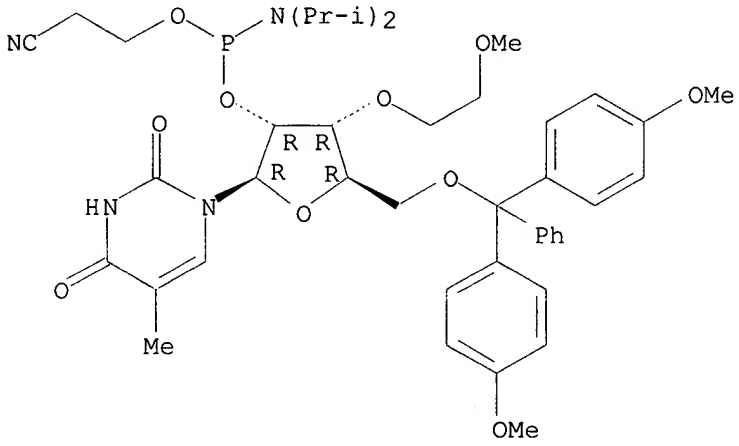
RN 170114-29-1 HCAPLUS
CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-O-[6-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)hexyl]-, 2'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



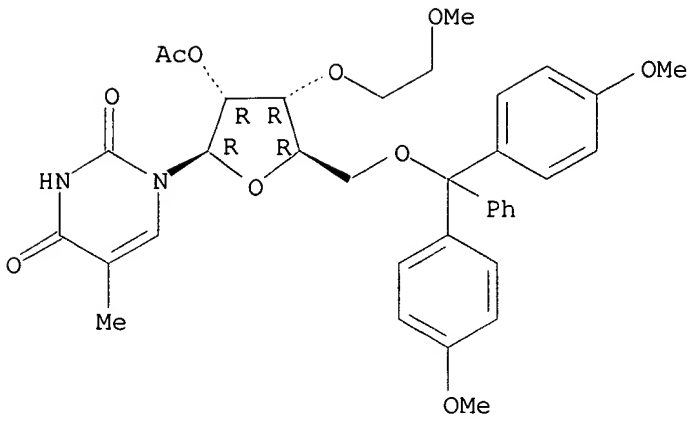
RN 256223-93-5 HCAPLUS
CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-O-(2-methoxyethyl)-5-methyl-, 2'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



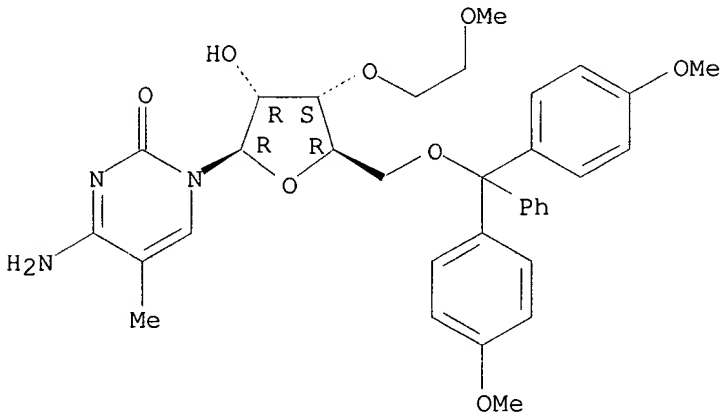
RN 256223-95-7 HCAPLUS
CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-O-(2-methoxyethyl)-5-methyl-, 2'-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



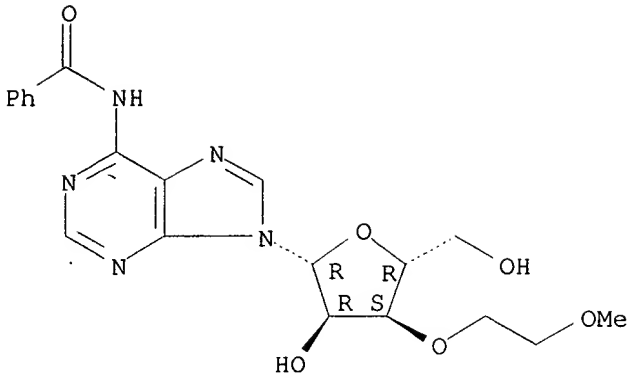

RN 256223-97-9 HCAPLUS
CN Cytidine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-O-(2-methoxyethyl)-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



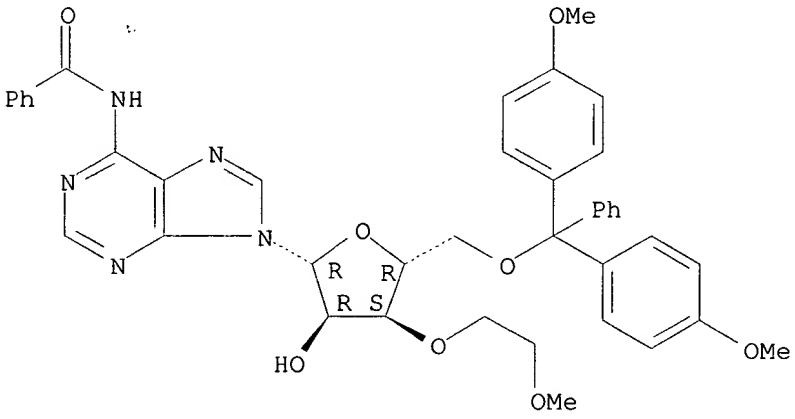

RN 256223-99-1 HCAPLUS
CN Adenosine, N-benzoyl-3'-O-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



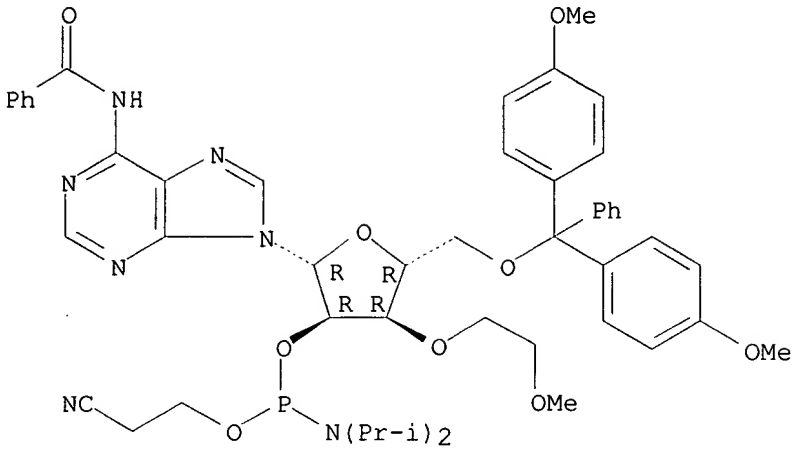
RN 256224-00-7 HCAPLUS
CN Adenosine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-O-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



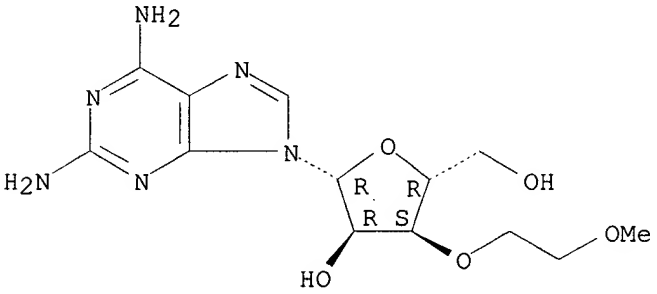
RN 256224-01-8 HCAPLUS
CN Adenosine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-O-(2-methoxyethyl)-, 2'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



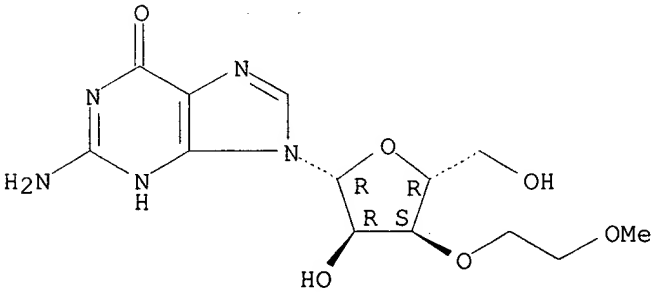
RN 256224-02-9 HCAPLUS
CN Adenosine, 2-amino-3'-O-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



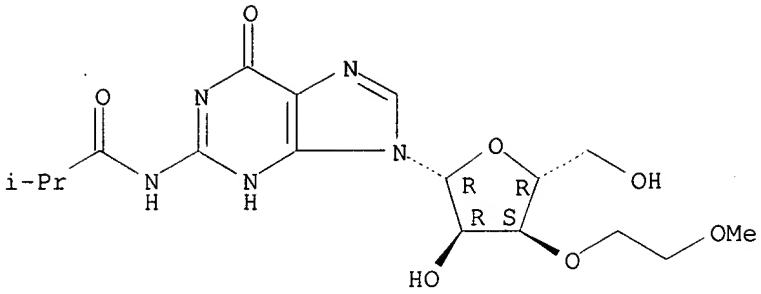
RN 256224-03-0 HCAPLUS
CN Guanosine, 3'-O-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



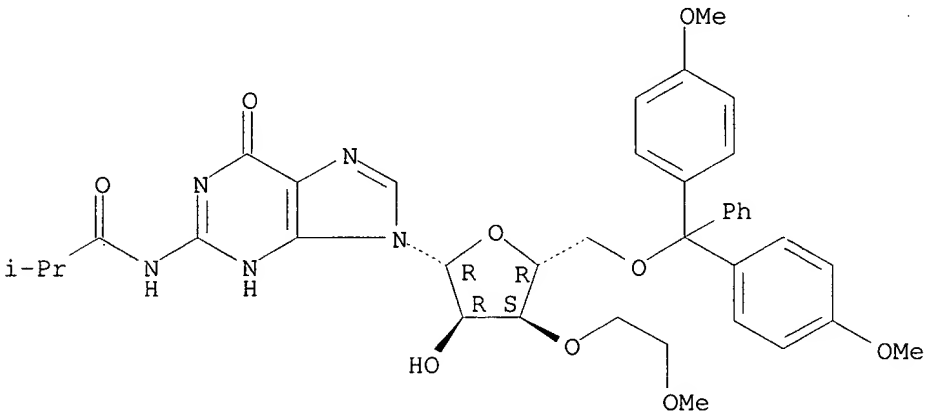
RN 256224-04-1 HCAPLUS
CN Guanosine, 3'-O-(2-methoxyethyl)-N-(2-methyl-1-oxopropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



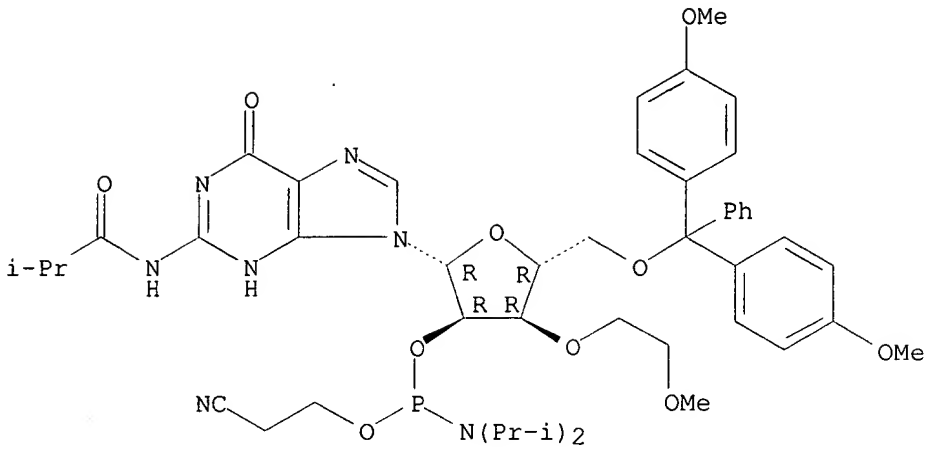
RN 256224-05-2 HCAPLUS
CN Guanosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-O-(2-methoxyethyl)-N-(2-methyl-1-oxopropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



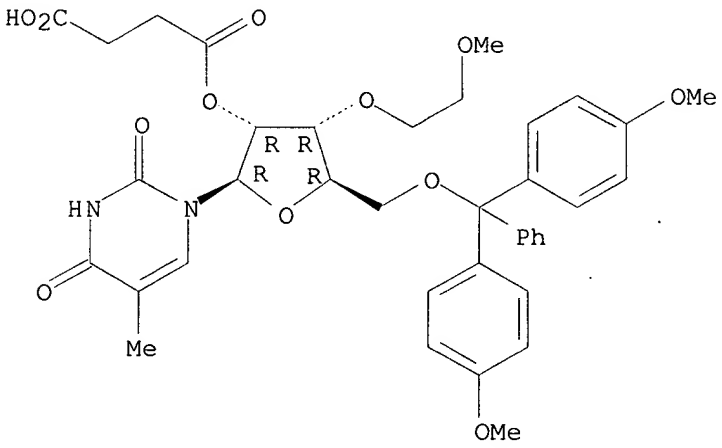
RN 256224-06-3 HCAPLUS
CN Guanosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-O-(2-methoxyethyl)-N-(2-methyl-1-oxopropyl)-, 2'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



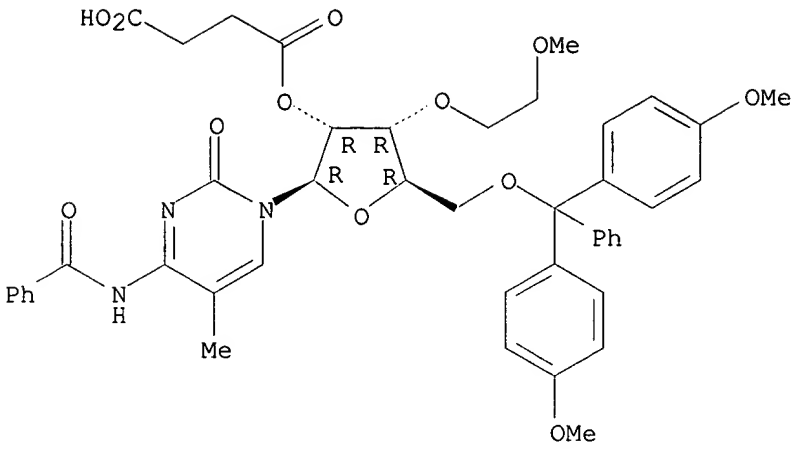
RN 256224-07-4 HCAPLUS
CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-O-(2-methoxyethyl)-5-methyl-, 2'-(hydrogen butanedioate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



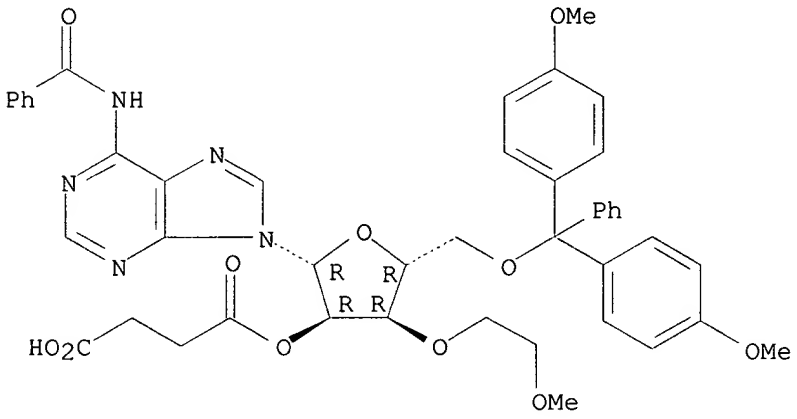
RN 256224-08-5 HCAPLUS
CN Cytidine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-(2-methoxyethyl)-5-methyl-, 2'-(hydrogen butanedioate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



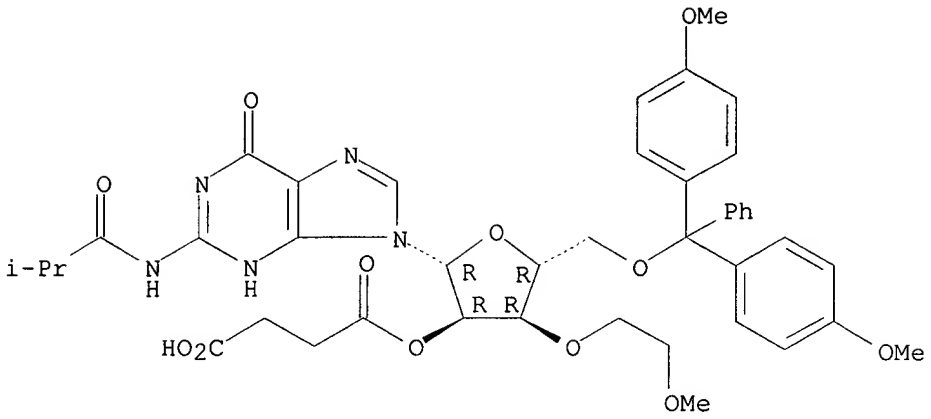
RN 256224-09-6 HCAPLUS
CN Adenosine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-(2-methoxyethyl)-, 2'-(hydrogen butanedioate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



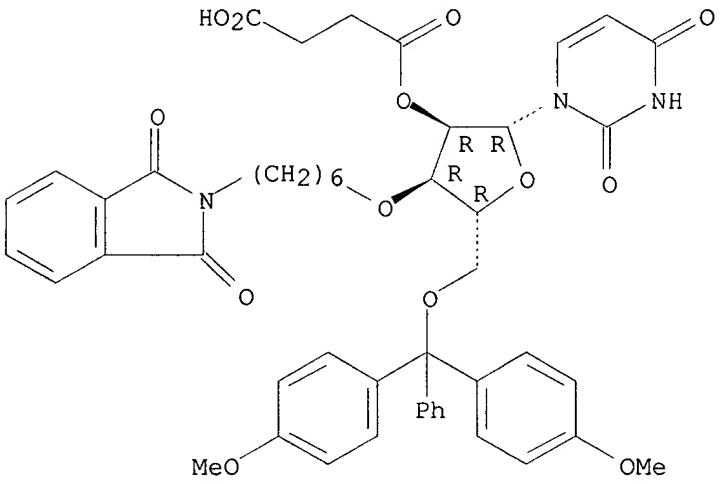
RN 256224-10-9 HCAPLUS
CN Guanosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-(2-methoxyethyl)-N-(2-methyl-1-oxopropyl)-, 2'-(hydrogen butanedioate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



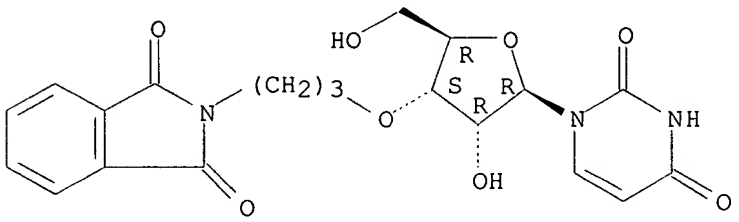
RN 256224-11-0 HCAPLUS
CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-3'-O-[6-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)hexyl]-, 2'-(hydrogen butanedioate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



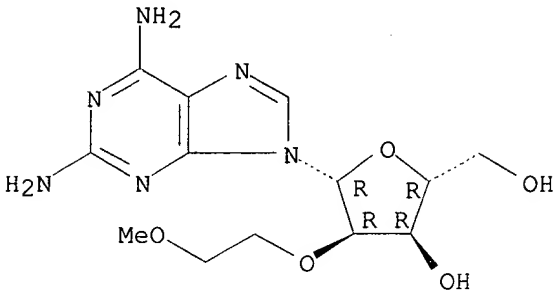
RN 256224-12-1 HCAPLUS
CN Uridine, 3'-O-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



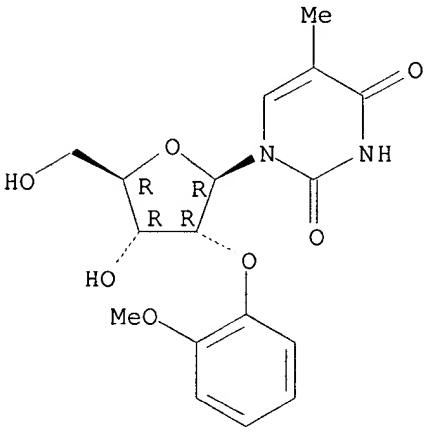
RN 256224-13-2 HCAPLUS
CN Adenosine, 2-amino-2'-O-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



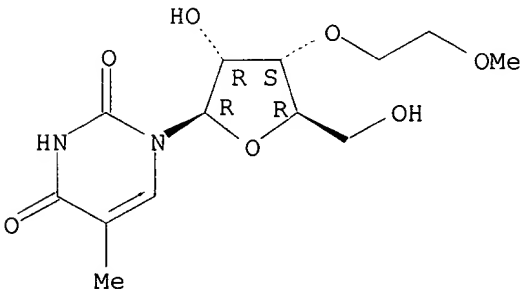
RN 256420-89-0 HCAPLUS
CN Uridine, 2'-O-(2-methoxyphenyl)-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 303197-29-7 HCAPLUS
CN Uridine, 3'-O-(2-methoxyethyl)-5-methyl- (9CI) (CA INDEX NAME)

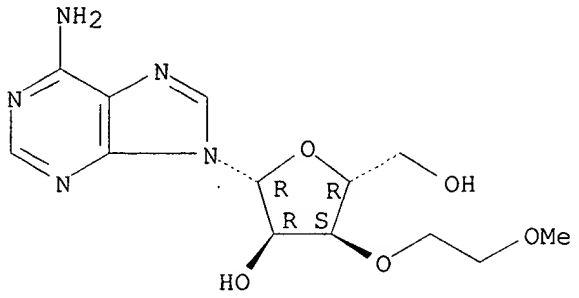
Absolute stereochemistry.



RN 303197-30-0 HCAPLUS

CN Adenosine, 3'-O-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ind

L15 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS
IC ICM C07H021-02
ICS C07H021-04
CC 33-10 (Carbohydrates)
Section cross-reference(s): 7, 22
ST oligonucleotide prepn **conformation** substrate RNase resistance nuclease
IT **Conformation**
(DNA; prepn. of oligonucleotides having A-DNA form and B-DNA form **conformational geometry** as substrates for RNase H and nuclease resistance)
IT Double stranded RNA
Oligonucleotides
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(prepn. of oligonucleotides having A-DNA form and B-DNA form **conformational geometry** as substrates for RNase H and nuclease resistance)
IT 9025-82-5, Phosphodiesterase
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(prepn. of oligonucleotides having A-DNA form and B-DNA form **conformational geometry** as substrates for RNase H and nuclease resistance)
IT 9026-81-7, Nuclease 80619-02-9, 5-Lipoxygenase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(prepn. of oligonucleotides having A-DNA form and B-DNA form **conformational geometry** as substrates for RNase H and nuclease resistance)
IT **149957-14-2P**, ISIS 2503 **181287-30-9P**
**216008-72-9P**, ISIS 14896 **216008-74-1P**, ISIS 14898
**216008-75-2P**, ISIS 14890 **216008-76-3P**, ISIS 14897
**216008-77-4P**, ISIS 14899 **216008-78-5P**, ISIS 13920
**256435-05-9P** **256435-06-0P** **256435-07-1P**
**303197-32-2P** **303197-33-3P** **303197-34-4P**

**304030-10-2P 304030-11-3P 304030-13-5P**
**304030-14-6P 304030-15-7P 304030-16-8P**
**304030-17-9P 304030-18-0P 304030-19-1P**
**304030-20-4P 304030-21-5P 304030-22-6P**
**304030-23-7P 304030-24-8P** 304030-25-9P
**304030-26-0P 304030-27-1P 304030-28-2P**
**304030-29-3P 304030-30-6P 304030-31-7P**
**304030-32-8P 304030-33-9P 304030-34-0P**
**304030-35-1P 304030-36-2P 304030-37-3P**
**304030-38-4P 304030-39-5P 304030-40-8P**
**304030-41-9P** 304030-42-0P **304486-97-3P**
**304705-19-9P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(prepn. of oligonucleotides having A-DNA form and B-DNA form **conformational geometry** as substrates for RNase H and nuclease resistance)

IT **58-61-7**, Adenosine, reactions 90-05-1, 2-Methoxyphenol 106-94-5, 1-Bromopropane 954-81-4, N-(5-Bromopentyl)phthalimide 1892-57-5, DEC 2127-10-8, DTNP 5394-18-3, N-(4-Bromobutyl)phthalimide 22423-26-3 24566-79-8, 6-Bromohexyl phthalimide 42822-78-6 **165381-50-0** 182495-84-7 **303197-31-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of oligonucleotides having A-DNA form and B-DNA form **conformational geometry** as substrates for RNase H and nuclease resistance)

IT **2096-10-8P 136834-10-1P 156881-42-4P**
**156881-43-5P 156881-44-6P 156881-45-7P**
**163759-49-7P 165381-01-1P 165381-32-8P**
**165381-39-5P 165381-41-9P 165381-44-2P**
**165381-45-3P 168427-74-5P 170114-29-1P**
**256223-93-5P 256223-95-7P 256223-97-9P**
**256223-99-1P 256224-00-7P 256224-01-8P**
**256224-02-9P 256224-03-0P 256224-04-1P**
**256224-05-2P 256224-06-3P 256224-07-4DP,**
LCA-CPG support **256224-08-5DP**, LCA-CPG support **256224-09-6DP**, LCA-CPG support **256224-10-9DP**, polymer support **256224-11-0DP**, aminopropyl-CPG support
**256224-12-1P 256224-13-2P 256420-89-0P**
**303197-29-7P 303197-30-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of oligonucleotides having A-DNA form and B-DNA form **conformational geometry** as substrates for RNase H and nuclease resistance)

cl 1 text search

KRISHNAN 09/970,971

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=> d que l32
L1          336 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MANOHARAN M?/AU
L2          224 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MOHAN V?/AU
L3          965 SEA FILE=HCAPLUS ABB=ON  PLU=ON  COOK P?/AU
L4          725 SEA FILE=HCAPLUS ABB=ON  PLU=ON  KAWASAKI A?/AU
L5         2114 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L1 OR L2 OR L3 OR L4)
L6       285937 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CONFORMATION?
L7          100 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L5 AND L6
L8           75 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CONFORMATIONAL GEOMETRY
L9            1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 AND L7
L18       74558 SEA FILE=HCAPLUS ABB=ON  PLU=ON  OLIGONUCLEOTIDES+NT1,NT2,BT1/C
                T
L20       23630 SEA FILE=HCAPLUS ABB=ON  PLU=ON  A"-"DNA
L21        3816 SEA FILE=HCAPLUS ABB=ON  PLU=ON  B"-"DNA
L22      518609 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CONFORMATION+ALL/CT
L23        4309 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L22 AND L18
L24         141 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L23 AND L20
L25         120 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L23 AND L21
L26          28 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L24 AND L25
L27         371 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20(P)L21
L29          27 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L26 NOT L9
L30          23 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L29 AND L27
L31      790806 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MAP OR MAPPING OR CLUSTER? OR
                CONTINUOUS?
L32           3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 AND L31
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=> d ibib abs

L32 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:12460 HCAPLUS
DOCUMENT NUMBER: 132:190939
TITLE: Sequence-dependent DNA Structure: Tetranucleotide Conformational **Maps**
AUTHOR(S): Packer, Martin J.; Dauncey, Mark P.; Hunter, Christopher A.
CORPORATE SOURCE: Krebs Institute for Biomolecular Science, Department of Chemistry, University of Sheffield, Sheffield, S3 7HF, UK
SOURCE: Journal of Molecular Biology (2000), 295(1), 85-103
CODEN: JMOBAK; ISSN: 0022-2836
PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A database of x-ray crystal structures of double helical DNA oligomers has been used to analyze the role of the sugar-phosphate backbone in coupling the conformational properties of neighboring dinucleotide steps. The base step parameters which are most strongly coupled to the backbone degrees of freedom are slide and shift, and these are the two dinucleotide step parameters which show strong correlations along a sequence: the value of slide follows the values in the neighboring steps, whereas shift tends to alternate. This conformational coupling is mediated by the shared furanose rings at the step junctions: a change in the value of slide causes a change in the mean value of the same strand 3' and 5'-.chi. torsion angle, and a change in the mean value of the 3' and 5' sugar pseudo-rotation phase angle, P; a change in the value of shift causes a difference between the same strand 3' and 5'-.chi. in **A-DNA** and a difference between the 3' and 5'-P in **B-DNA**. We have used a database of tetranucleotide x-ray crystal structures to parameterize a simple model for the coupling of slide and shift. Using this junction model together with our dinucleotide step potential energy **maps** described previously, we can in principle calc. the structure of any DNA oligomer. The parameterization indicates that the rotational step parameters are accurate to within 5.degree., and the translational step parameters are accurate to within 0.5 .ANG.. The model has been used to study the potential energy surfaces of all possible tetranucleotide sequences, and the calcns. agree well with the exptl. data from x-ray crystal structures. Some dinucleotide steps are context independent (AA/TT, AT and TA), because the conformational properties of all possible neighboring steps are compatible. When the conformational properties of the neighbors are not compatible, the behavior of a step cannot be understood at the dinucleotide level. Thus the conformations of CG, GC and GG/CC are all strongly context dependent. The remaining mixed sequence steps show weakly context-dependent behavior. The approach allows the calcn. of the relative stability and flexibility of tetranucleotide sequences, and the results indicate why TATA is used as an origin of replication. Clear predictions are made about sequences which have not yet been characterized crystallog. In particular, poly(CCA).cntdot.poly(TGG) is predicted to have an unusual structure which lies between the C and D-DNA polymorphs. (c) 2000 Academic Press.
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ind

L32 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2002 ACS
CC 6-2 (General Biochemistry)
ST DNA structure prediction tetranucleotide conformational **map**
IT **Conformation**
**Helix (conformation)**
(DNA; tetranucleotide conformational **maps** and prediction of sequence-dependent DNA structure)
IT Genetic element
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(TATA box; tetranucleotide conformational **maps** and prediction of sequence-dependent DNA structure)
IT Conformational potential energy surface
DNA sequences
Molecular modeling
(tetranucleotide conformational **maps** and prediction of sequence-dependent DNA structure)
IT DNA
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(tetranucleotide conformational **maps** and prediction of sequence-dependent DNA structure)
IT **Nucleotides, biological studies**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(tetranucleotides; tetranucleotide conformational **maps** and prediction of sequence-dependent DNA structure)

=> d ibib abs 2

L32 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:117310 HCAPLUS
DOCUMENT NUMBER: 128:267317
TITLE: A self-organizing feature **map** for **clustering** nucleic acids. Application to a data matrix containing **A-DNA** and **B-DNA** dinucleotides
AUTHOR(S): Beckers, M. L. M.; Melssen, W. J.; Buydens, L. M. C.
CORPORATE SOURCE: Laboratory for Analytical Chemistry, Faculty of Science, University of Nijmegen, Nijmegen, 6525 ED, Neth.
SOURCE: Computers & Chemistry (Oxford) (1998), Volume Date 1997, 21(6), 377-390
CODEN: COCHDK; ISSN: 0097-8485
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A self-organizing feature **map** to **cluster** DNA dinucleotides is presented. During a training session 244 training. patterns, each consisting of nine torsion angles, are **clustered** in a 10 by 10 **map**. The method is successful for sepg. the four known DNA classes in the training set. Contour plots of the wts. after a training session indicate gradients in torsion angles corresponding to class sepn. Moreover, certain units in the **map** probably correspond to unfavorable torsion angle combinations resulting in, e.g. van der Waals clashes. Hence, although no direct relation to a conformation's energy (as in a Ramachandran plot) is present in the-**map**, it-may provide a multidimensional interpretation of accessible and forbidden areas for dinucleotides. The applicability of the method on this DNA data matrix shows its potential to be used in more extensive structural anal. studies, e.g. in a case of comparing DNA with RNA. Several test patterns resulting from mols. with unusual structural characteristics are identified with the **map**.

=> d ind 2

L32 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2002 ACS
CC 6-2 (General Biochemistry)
ST DNA dinucleotide **clustering** conformation
IT **Conformation**
(DNA; self-organizing feature **map** for **clustering** nucleic acids and its application to a data matrix contg. **A-DNA** and **B-DNA** dinucleotides)
IT **Oligonucleotides**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(dinucleotides; self-organizing feature **map** for **clustering** nucleic acids and its application to a data matrix contg. **A-DNA** and **B-DNA** dinucleotides)
IT DNA
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(self-organizing feature **map** for **clustering** nucleic acids and its application to a data matrix contg. **A-DNA** and **B-DNA** dinucleotides)

=> d ibib abs 3

L32 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:83918 HCAPLUS
DOCUMENT NUMBER: 104:83918
TITLE: Raman spectra of single crystals of r(GCG)d(CGC) and d(CCCCGGGG) as models for **A DNA**, their structure transitions in aqueous solution, and comparison with double-helical poly(dG).cntdot.poly(dC)
AUTHOR(S): Benevides, J. M.; Wang, A. H. J.; Rich, A.; Kyogoku, Y.; Van der Marel, G. A.; Van Boom, J. H.; Thomas, G. J., Jr.
CORPORATE SOURCE: Dep. Chem., Southeast. Massachusetts Univ., North Dartmouth, MA, 02747, USA
SOURCE: Biochemistry (1986), 25(1), 41-50
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The double-stranded oligonucleotides [r(GGG)d(CGC)]2 and [d(CCCCGGGG)]2 in single-crystal and soln. forms were investigated by Raman spectroscopy. Comparison of the Raman spectra with results of single-crystal x-ray diffraction and with data from polynucleotides permits the identification of a no. of Raman frequencies diagnostic of the A-helix structure for GC sequences. The guanine ring frequency characteristic of C3'-endo pucker and anti base orientation is assigned at 668 cm-1 for both deoxyriboguanosine and riboguanosine residues of the DNA/RNA hybrid [r(GGG)d(CGC)]2. The A-helix backbone of cryst. [r(GCG)d(CGC)2] is altered slightly in the aq. structure, consistent with the conversion of .gtoreq.2 residues to the C2'-endo pucker sandwiched between terminal and penultimate pairs of C3'-endo pucker. The A-A-B-A-B-A-A-A backbone of the cryst. octamer is converted completely to a **B-DNA** fragment in aq. soln. with Raman markers characteristic of the 3'-endo-anti-guanosine (682) and the B backbone (826 cm-1). In the case of poly(dG).cntdot.poly(dC), considerable structural variability is detected. A 4% soln. of the duplex is largely **A DNA**, but a 2% soln. is predominantly **B DNA**. On the other hand, an oriented fiber drawn at 75% relative humidity reveals Raman markers characteristic of both **A DNA** and a modified **B DNA**, not unlike the [d(CCCCGGGG)]2 crystal. A comparison of Raman and CD spectra of the [d(CCCCGGGG)]2 and poly(dG).cntdot.poly(dC) structures suggests the need for caution in the interpretation of CD data from guanosine **clusters** in DNA.

=> d ind 3

L32 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2002 ACS
CC 6-2 (General Biochemistry)
Section cross-reference(s): 73, 75
ST oligonucleotide crystal conformation Raman; DNA model conformation Raman; polydeoxyribonucleotide conformation Raman
IT Salt effect
(conformation of DNA models response to)
IT **Nucleotides, properties**
RL: PRP (Properties)
(conformation of, in DNA models, Raman spectra in relation to)
IT Deoxyribonucleic acids
Ribonucleic acids

RL: BIOL (Biological study)
(double-stranded, Raman spectra of models of)
IT Circular dichroism
(of double-stranded oligodeoxyribonucleosides, DNA in relation to)
IT Raman spectra
(of oligo- and polynucleosides, DNA in relation to)
IT **Conformation and Conformers**
(of oligo- and polynucleosides, Raman spectra in relation to)
IT 25512-84-9
RL: PRP (Properties)
(conformation of, Raman spectra in relation to)
IT 99327-09-0 99327-10-3
RL: BIOL (Biological study)
(double-stranded, conformation of crystals and soln. forms of, Raman spectra in relation to)

Claim 1 text search

KRISHNAN 09/970,971

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=> d que l33
L1          336 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MANOHARAN M?/AU
L2          224 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MOHAN V?/AU
L3          965 SEA FILE=HCAPLUS ABB=ON  PLU=ON  COOK P?/AU
L4          725 SEA FILE=HCAPLUS ABB=ON  PLU=ON  KAWASAKI A?/AU
L5         2114 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L1 OR L2 OR L3 OR L4)
L6       285937 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CONFORMATION?
L7          100 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L5 AND L6
L8           75 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CONFORMATIONAL GEOMETRY
L9            1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 AND L7
L18       74558 SEA FILE=HCAPLUS ABB=ON  PLU=ON  OLIGONUCLEOTIDES+NT1,NT2,BT1/C
                T
L20       23630 SEA FILE=HCAPLUS ABB=ON  PLU=ON  A"-"DNA
L21        3816 SEA FILE=HCAPLUS ABB=ON  PLU=ON  B"-"DNA
L22      518609 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CONFORMATION+ALL/CT
L23        4309 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L22 AND L18
L24         141 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L23 AND L20
L25         120 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L23 AND L21
L26          28 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L24 AND L25
L27         371 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20(P)L21
L29          27 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L26 NOT L9
L30          23 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L29 AND L27
L31      790806 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MAP OR MAPPING OR CLUSTER? OR
                CONTINUOUS?
L32           3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 AND L31
L33          20 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 NOT L32
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=> d ibib abs 1

L33 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:109276 HCAPLUS
DOCUMENT NUMBER: 130:308031
TITLE: Structure of the d(CGCCCGCGGGCG) Dodecamer: A Kinked **A-DNA** Molecule Showing Some **B-DNA** Features
AUTHOR(S): Malinina, Lucy; Fernandez, Luzimar G.; Huynh-Dinh, Tam; Subirana, Juan A.
CORPORATE SOURCE: Departament d'Enginyeria Quimica, E.T.S.E.I.B., Barcelona, 08028, Spain
SOURCE: Journal of Molecular Biology (1999), 285(4), 1679-1690
CODEN: JMOBAK; ISSN: 0022-2836
PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have detd. the structure of the dodecamer duplex d(CGCCCGCGGGCG)2. A careful use of the mol. replacement program AMoRe has been essential in order to solve the structure. This dodecamer shows a unique conformation, quite different from all the previously studied oligonucleotide duplexes: the central octamer has an A conformation, but with a sharp 65 .degree. kink in the center; the terminal base-steps have a B-like conformation; the major groove is completely closed in the center, a hollow mol. is thus found. The results obtained confirm the high degree of variability of DNA structure. A new type of kink and an intermediate A/B double-helical conformation have been found. Such intermediate conformation differs from those described in DNA polymerase complexes. (c) 1999 Academic Press.
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ind

L33 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2002 ACS
CC 6-2 (General Biochemistry)
Section cross-reference(s): 75
ST DNA conformation kink A B
IT **Conformation**
(A form; kinked A conformation with some B conformation features of dodecamer duplex d(CGCCCGCGGGCG))
IT **Conformation**
(B form; kinked A conformation with some B conformation features of dodecamer duplex d(CGCCCGCGGGCG))
IT **Conformation**
(DNA; kinked A conformation with some B conformation features of dodecamer duplex d(CGCCCGCGGGCG))
IT **Conformational transition**
**Crystal structure**
(kinked A conformation with some B conformation features of dodecamer duplex d(CGCCCGCGGGCG))
IT DNA
**Oligodeoxyribonucleotides**
RL: PRP (Properties)
(kinked A conformation with some B conformation features of dodecamer duplex d(CGCCCGCGGGCG))
IT 223455-79-6
RL: PRP (Properties)
(kinked A conformation with some B conformation features of dodecamer

duplex d(CGCCCGCGGGCG))

=> d ibib abs ind 2

L33 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:468633 HCAPLUS
DOCUMENT NUMBER: 127:201553
TITLE: Structure of **a DNA** analog of the primer for HIV-1 RT second strand synthesis
AUTHOR(S): Han, Gye Won; Kopka, Mary L.; Cascio, Duilio; Grzeskowiak, Kazimierz; Dickerson, Richard E.
CORPORATE SOURCE: Molecular Biology Institute, University California at Los Angeles, Los Angeles, CA, 90095, USA
SOURCE: Journal of Molecular Biology (1997), 269(5), 811-826
CODEN: JMOBAK; ISSN: 0022-2836
PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The non-self-complementary DNA decamer CAAAGAAAAG.cntdot.CTTTTCTTTG is **a DNA**/DNA analog of a portion of the polypurine tract or PPT, which is a RNA/DNA hybrid that serves as a primer for synthesis of the (+) DNA strand by HIV reverse transcriptase (RT), and which is not digested by the RNase H domain of reverse transcriptase following (-) strand synthesis. The same unusual conformation that eludes RNase H, thought to be a change in width of minor groove, may also be responsible for the inhibition of HIV RT by minor groove binding drugs such as distamycin and their bis-linked derivs. The present X-ray crystal structure of this DNA decamer exhibits the usual properties of A-tract **B-DNA** under biol. relevant conditions: large propeller twist of base-pairs, narrowed minor groove, and a straight helix axis. Groove narrowing is fully developed in the A-A-A-A region, but not in the A-A-A region, which previous investigators have proposed as being too short to exhibit typical A-tract properties. The RNA/DNA hybrid produced by HIV reverse transcriptase during (-) strand synthesis presumably forms a "heteromerous" or H-helix with narrower minor groove than an A-helical RNA/RNA duplex. If the narrowing of minor groove in A-tract H-helixes is comparable to that seen in A-tract B-helixes, then the narrowed minor groove of the polypurine tract could make the second primer site both (1) impervious to RNase H digestion, and (2) susceptible to inhibition by minor groove binding drugs.

CC 6-2 (General Biochemistry)
Section cross-reference(s): 75

ST crystal structure DNA analog primer HIV1; reverse transcriptase primer DNA structure HIV1; virus HIV1 PPT DNA analog structure

IT **Conformation**
(B form, A-tract; crystal structure of DNA analog of primer for HIV-1 reverse transcriptase second strand synthesis)

IT Primers (nucleic acid)
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(HIV-1 reverse transcriptase; crystal structure of DNA analog of primer for HIV-1 reverse transcriptase second strand synthesis)

IT Genetic element
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(PPT (polypurine tract); crystal structure of DNA analog of primer for HIV-1 reverse transcriptase second strand synthesis)

IT **Oligodeoxyribonucleotides**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(crystal structure of DNA analog of primer for HIV-1 reverse

transcriptase second strand synthesis)

IT **Crystal structure**
(of DNA analog of primer for HIV-1 reverse transcriptase second strand synthesis)

IT Human immunodeficiency virus 1
(structure of DNA analog of primer for HIV-1 reverse transcriptase second strand synthesis)

IT 9068-38-6
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(crystal structure of DNA analog of primer for HIV-1 reverse transcriptase second strand synthesis)

IT 194741-81-6
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(crystal structure of; DNA analog of primer for HIV-1 reverse transcriptase second strand synthesis)

=> d ibib abs ind 3

L33 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:234206 HCAPLUS
DOCUMENT NUMBER: 122:49319
TITLE: Hydrogen bonding of nucleotide base pairs: application of the PM3 method
AUTHOR(S): Lively, Tricia N.; Jurema, Marcus W.; Shields, George C.
CORPORATE SOURCE: Dep. Chem., Lake Forest Coll., Lake Forest, IL, 60045, USA
SOURCE: International Journal of Quantum Chemistry, Quantum Biology Symposium (1994), 21(Proceedings of the International Symposium on the Application of Fundamental Theory to Problems of Biology and Pharmacology, 1994), 95-107
CODEN: IJQBDZ; ISSN: 0360-8832
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The ability of the PM3 semiempirical quantum mech. method to reproduce hydrogen bonding in nucleotide base pairs was assessed. Results of PM3 calcns. on the nucleotides 2'-deoxyadenosine 5'-monophosphate (pdA), 2'-deoxyguanosine 5'-monophosphate (pdG), 2'-deoxycytidine 5'-monophosphate (pdC), and 2'-deoxythymidine 5'-monophosphate (pdT) and the base pairs pdA-pdT, pdG-pdC, and pdG(syn)-pdC are presented and discussed. The PM3 method is the first of the parameterized NDDO quantum mech. models with any ability to reproduce hydrogen bonding between nucleotide base pairs. Intermol. hydrogen bond lengths between nucleotides displaying Watson-Crick base pairing are 0.1-0.2 .ANG. less than exptl. results. Nucleotide bond distances, bond angles, and torsion angles about the glycosyl bond (.chi.), the C4'-C5' bond (.gamma.), and the C5'-O5' bond (.beta.) agree with exptl. results. There are many possible conformations of nucleotides. PM3 calcns. reveal that many of the most stable conformations are stabilized by intramol. C-H---O hydrogen bonds. These interactions disrupt the usual sugar puckering. The stacking interactions of a dT-pdA duplex are examd. at different levels of gradient optimization. The intramol. hydrogen bonds found in the nucleotide base pairs disappear in the duplex, as a result of the addnl. constraints on the phosphate group when part of **a DNA** backbone. Sugar puckering is reproduced by the PM3 method for the four bases in the dT-pdA duplex. PM3 underestimates the attractive stacking interactions of base pairs in a **B-DNA** helical conformation. The performance of the PM3 method implemented in SPARTAN is contrasted with that implemented in MOPAC. At present, accurate ab initio calcns. are too time-consuming to be of practical use, and mol. mechanics methods cannot be used to det. quantum mech. properties such as reaction-path calcns., transition-state structures, and activation energies. The PM3 method should be used with extreme caution for examn. of small DNA systems. Future parameterizations of semiempirical methods should incorporate base stacking interactions into the parameterization data set to enhance the ability of these methods.

CC 6-2 (General Biochemistry)
Section cross-reference(s): 9, 33, 65
ST hydrogen bonding nucleotide base pair PM3
IT **Conformation and Conformers**
Hydrogen bond
(PM3 quantum mech. study of hydrogen bonding of nucleotide base pairs)
IT Nucleic acid bases

RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(PM3 quantum mech. study of hydrogen bonding of nucleotide base pairs)

IT Deoxyribonucleic acids
RL: PRP (Properties)
(PM3 quantum mech. study of hydrogen bonding of nucleotide base pairs)

IT **Nucleotides, biological studies**
RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(deoxyribo-, PM3 quantum mech. study of hydrogen bonding of nucleotide base pairs)

IT Hydrogen bond
(intramol., PM3 quantum mech. study of hydrogen bonding of nucleotide base pairs)

IT Molecular orbital
(third-parametric (PM3), PM3 quantum mech. study of hydrogen bonding of nucleotide base pairs)

IT 365-07-1, 2'-Deoxythymidine 5'-monophosphate 653-63-4, 2'-Deoxyadenosine 5'-monophosphate 902-04-5, 2'-Deoxyguanosine 5'-monophosphate 1032-65-1, 2'-Deoxycytidine 5'-monophosphate
RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(PM3 quantum mech. study of hydrogen bonding of nucleotide base pairs)

=> d ibib abs ind 4

L33 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:238435 HCAPLUS
DOCUMENT NUMBER: 120:238435
TITLE: 2D 1H and 31P NMR spectra and distorted **A-DNA**-like duplex structure of a phosphorodithioate oligonucleotide
AUTHOR(S): Cho, Yesun; Zhu, Frank C.; Luxon, Bruce A.; Gorenstein, David G.
CORPORATE SOURCE: Dep. Chem., Purdue Univ., West Lafayette, IN, 47907, USA
SOURCE: J. Biomol. Struct. Dyn. (1993), 11(3), 685-702
CODEN: JBSDD6; ISSN: 0739-1102
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Assignment of the 1H and 31P NMR spectra of a phosphorodithioate modified oligonucleotide decamer duplex, d(CGCTTpS2-AAGCG)2 (10-mer-S; a site of dithioate substitution is designated with the symbols pS2-), was achieved by two-dimensional homonuclear TOCSY, NOESY and 1H-31P Pure Absorption phase Const. time (PAC) heteronuclear correlation spectroscopy. In contrast to the parent palindromic decamer sequence which has been shown to exist entirely in the duplex **B-DNA** conformation under comparable conditions (100 mM KCl), the dithiophosphate analog forms a hairpin loop. However, the duplex form of the the dithioate oligonucleotide can be stabilized at lower temps., higher salt and strand concn. The soln. structure of the decamer duplex was calcd. by an iterative hybrid relaxation matrix method (MORASS) combined with 2D NOESY-distance restrained mol. dynamics. These backbone modified compds., potentially attractive antisense oligonucleotide agents, are often assumed to possess similar structure as the parent nucleic acid complex. Importantly, the refined structure of the phosphorodithioate duplex shows a significant deviation from the parent unmodified, phosphoryl duplex. An overall bend and unwinding in the phosphorodithioate duplex is obsd. The structural distortion of the phosphorodithioate duplex was confirmed by comparison of helicoidal parameters and groove dimensions. Esp., the helical twists of the phosphorodithioate decamer deviate significantly from the parent phosphoryl decamer. The minor groove width of phosphorodithioate duplex 10-mer-S varies between 8.4 and 13.3 .ANG. which is much wider than those of the parent phosphoryl decamer d(CGCTTAAGCG)2 (4.2.apprx.9.4 .ANG.). The larger minor groove width of 10-mer-S duplex contributes to the unwinding of the backbone and indicates that the duplex has an overall **A-DNA**-like conformation in the region surrounding the dithiophosphate modification.

CC 6-2 (General Biochemistry)
ST DNA phosphorodithioate conformation NMR; phosphorodithioate oligonucleotide conformation NMR
IT **Conformation and Conformers**
(**A**, of phosphorodithioate oligonucleotide duplex)
IT **Conformation and Conformers**
(**hairpin loop**, of phosphorodithioate oligonucleotide, in low salt)
IT **Nucleotides, polymers**
RL: BIOL (Biological study)
(**oligo-, deoxyribo-, thiophosphate-linked**, conformation A-like structure of duplex, NMR study of)
IT Functional groups
(phosphorothiodiester, DNA structural response to)
IT Deoxyribonucleic acids

RL: BIOL (Biological study)
(thiophosphate-linked, conformation A-like structure of duplex, NMR study of)

IT 130408-67-2
RL: PRP (Properties)
(hairpin conformation of, in low salt)

IT 154304-91-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and distorted **A-DNA**-like conformation of)

=> d ibib abs ind 5

L33 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:99678 HCAPLUS
DOCUMENT NUMBER: 120:99678
TITLE: Spatial translational motions of base pairs in DNA molecules: application of the extended matrix generator method
AUTHOR(S): Marky, Nancy L.; Olson, Wilma K.
CORPORATE SOURCE: Dep. Chem., Rutgers, State Univ., New Brunswick, NJ, 08903, USA
SOURCE: Biopolymers (1994), 34(1), 121-42
CODEN: BIPMAA; ISSN: 0006-3525
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors have used the elementary generator matrixes outlined in the preceding paper to examine the conformational plasticity of the nucleic acid double helix. Here the authors investigate kinked DNA structures made up of alternating B- and A-type helixes and intrinsically curved duplexes perturbed by the intercalation of ligands. The authors model the B-to-A transition by the lateral translation of adjacent base pairs, and the intercalation of ligands by the vertical displacement of neighboring residues. The authors report a complete set of av. configuration-dependent parameters, ranging from scalars (i.e., persistence lengths) to first- and second-order tensor parameters (i.e., av. second moments of inertia), as well as approxns. of the assocd. spatial distributions of the DNA and their angular correlations. The av. structures of short chains (of lengths less than 100 base pairs) with local kinks or intrinsically curved sequences are essentially rigid rods. At the smallest chain lengths (10 base pairs), the kinked and curved chains exhibit similar av. properties, although they are structurally perturbed compared to the std. **B-DNA** duplex. In contrast, at lengths of 200 base pairs, the curved and kinked chains are more compact on av. and are located in a different space from the std. B- or **A-DNA** helix. While **A-DNA** is shorter and thicker than **B-DNA** in x-ray models, the long flexible **A-DNA** helix is thinner and more extended on av. than its **B-DNA** counterpart because of more limited fluctuations in local structure. Curved polymers of 50 base pairs or longer also show significantly greater asymmetry than other DNAs (in terms of the distribution of base pairs with respect to the center of gravity of the chain). The intercalation of drugs in the curved DNA straightens and extends the smoothly deformed template. The dimensions of the av. ellipsoidal boundaries defining the configurations of the intercalated polymers are roughly double those of the intrinsically curved chain. The altered proportions and orientations of these d. functions reflect the changing shape and flexibility of the double helix. The calcns. shed new light on the possible structural role of short **A-DNA** fragments in long B-type duplexes and also offer a model for understanding how GC-specific intercalative ligands can straighten naturally curved DNA. The mechanism is not immediately obvious from current models of DNA curvature, which attribute the bending of the chain to a perturbed structure in repeating tracts of A.cntdot.T base pairs.

CC 6-2 (General Biochemistry)
ST DNA base pair translational motion conformation
IT Ligands
RL: BIOL (Biological study)
(DNA intercalation with, conformation response to, base pair spatial translational motions in)

IT Deoxyribonucleic acids
RL: BIOL (Biological study)
(base pairs in, spatial translational motions of, extended matrix generator method for study of)
IT Chains, chemical
(length of, of DNA, structure in relation to)
IT **Conformation and Conformers**
(of DNA, base pair spatial translational motions in, **extended** matrix generator method for study of)
IT Nucleic acid bases
RL: BIOL (Biological study)
(pairs of, spatial translational motion of, of DNA, extended matrix generator method for study of)
IT **Nucleotides, polymers**
RL: BIOL (Biological study)
(**oligo-**, **deoxyribo-**, conformation of and spatial translational motions of base pairs in)
IT 65-71-4, Thymine
RL: PRP (Properties)
(base pair with adenine, spatial translational motion of, of DNA, extended matrix generator method for study of)
IT 73-40-5, Guanine
RL: PRP (Properties)
(base pair with cytosine, spatial translational motion of, of DNA, extended matrix generator method for study of)
IT 71-30-7, Cytosine
RL: PRP (Properties)
(base pair with guanine, spatial translational motion of, of DNA, extended matrix generator method for study of)
IT 73-24-5, Adenine, biological studies
RL: BIOL (Biological study)
(base pair with thymine, spatial translational motion of, of DNA, extended matrix generator method for study of)

=> d ibib abs ind 6

L33 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1993:489139 HCAPLUS
DOCUMENT NUMBER: 119:89139
TITLE: Structural influence of RNA incorporation in DNA: Quantitative nuclear magnetic resonance refinement of d(CG)r(CG)d(CG) and d(CG)r(C)d(TAGCG)
AUTHOR(S): Jaishree, T. N.; van der Marel, Gijs A.; van Boom, Jacques H.; Wang, Andrew H. J
CORPORATE SOURCE: Dep. Cell Struct. Biol., Univ. Illinois, Urbana, IL, 61801, USA
SOURCE: Biochemistry (1993), 32(18), 4903-11
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB RNA and DNA adopt different types of conformations, i.e., A-type with C3'-endo sugar pucker for RNA and B-type with C2'-endo sugar pucker for DNA, resp. The structural influence of the incorporation of RNA nucleotides into DNA is less understood. In this paper, the authors present the three-dimensional structures of two RNA-contg. oligonucleotides, d(CG)r(CG)d(CG) and d(CG)r(C)d(TAGCG), as detd. by the NMR refinement procedure, and assess the possible structural perturbation of DNA induced by RNA. With a single RNA insertion into an octamer DNA, its overall conformation remains as the canonical **B-DNA**, except that the sugar pucker of the rC3 residue is C3'-endo (pseudorotation angle P = 3.6.degree.). In contrast, the hybrid hexamer is neither the pure **B-DNA** nor the pure **A-DNA** conformation. Instead, a model is proposed in which the DNA parts adopt B conformation, whereas the RNA part adopts A conformation, with the overall conformation closer to **A-DNA**. To ensure an exhaustive search of the conformational space, the model was subjected to 100-ps simulated annealing with slow cooling or 100-ps mol. dynamics with subsequent quenching. Models obtained at different time points of the trajectories were further subjected to the SPEDREF NOE refinement and they appeared to arrive at a convergent model (<0.5 .ANG. root mean square deviation for the central four base pairs). The consensus hexamer structure contains a significant discontinuity at the (rG4)p(dC5) step with a base pair tilt angle of 6.7.degree. and roll angle of 11.5.degree.. This discontinuity may be related to the structural "bend" that occurs at the junction of the RNA and DNA helices.

CC 6-2 (General Biochemistry)
Section cross-reference(s): 73
ST conformation DNA RNA hybrid NMR
IT Ribonucleic acids
RL: BIOL (Biological study)
(-DNA hybrids, conformation of, length of RNA effect on, NMR study of)
IT Deoxyribonucleic acids
RL: BIOL (Biological study)
(-RNA hybrids, conformation of, length of RNA effect on, NMR study of)
IT Nuclear magnetic resonance
(of DNA-RNA hybrids)
IT **Conformation and Conformers**
(of DNA-RNA hybrids, length of RNA inserts effect on, NMR study of)
IT **Conformation and Conformers**
(**A**, of RNA of DNA-RNA hybrid)
IT **Conformation and Conformers**
(**B**, of DNA, of DNA-RNA hybrid)
IT **Nucleotides, polymers**

RL: PRP (Properties)
(**oligo**-, (**deoxyribo**-ribo)-, conformation of, length of RNA insert effect on, NMR study of)

IT 121013-49-8 147977-01-3
RL: PRP (Properties)
(conformation of, NMR study of)

=> d ibib abs ind 7

L33 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1993:207730 HCAPLUS
DOCUMENT NUMBER: 118:207730
TITLE: Nuclear magnetic resonance study of a deoxyoligonucleotide duplex containing a three base bulge
AUTHOR(S): Aboul-Ela, Fareed; Murchie, Alastair I. H.; Homans, Steven W.; Lilley, David M. J.
CORPORATE SOURCE: Dep. Biochem., Univ. Dundee, Dundee, DD1 4HN, UK
SOURCE: J. Mol. Biol. (1993), 229(1), 173-8
CODEN: JMOBAK; ISSN: 0022-2836
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The three-dimensional structure of **a DNA** oligonucleotide contg. three extra unpaired adenosine residues (dGCCAGGAAATCGGAC + dGTCCGACCTGGC) and that of the perfect duplex analog (dGCCAGGTCGGAC + dGTCCGACCTGGC) have been studied in soln. by 1H and 13C NMR. All nonexchangeable arom. and H-1', H-2', H-2'' sugar protons were assigned using std. assignment pathways for **B-DNA**. All cross-peaks within these pathways were present for the perfect duplex mol. as would be expected for a right-handed A- or B-form duplex. However, a few cross-peaks which would be expected in the std. case are extremely weak in the nuclear Overhauser enhancement spectroscopy (NOESY) spectrum of the bulged duplex even at long mixing times (250 ms). For example, almost no cross-relaxation is obsd. between the H-6 proton of C22 and the H-1' of A21, directly across from the three base bulge. Yet the continuity of assignment pathways through the three base bulge argues against any discontinuous looping out of one or more of the extra adenosine residues. Double quantum-filtered correlated spectroscopy expts. demonstrate very little deviation from south sugar conformations from residues at or near the bulge. The perfect duplex contains three A.cntdot.T base pairs as expected, resulting in three very intense T imino-AH2 cross-peaks in the H2O NOESY expt. In contrast, only two such intense cross-peaks are obsd. in the same expt. using the bulged duplex sample. Assignments of the two T imino peaks using one-dimensional NOEs are consistent with disruption of the T.cntdot.A base-pair immediately 3' to the bulge; this is consistent with the earlier observation of chem. reactivity at a T 3' to an An or Tn bulge. Evidence of disruption of the G.cntdot.C base-pair immediately 5' to the bulge was also found.

CC 6-2 (General Biochemistry)
Section cross-reference(s): 77
ST bulge DNA conformation NMR
IT Deoxyribonucleic acids
RL: BIOL (Biological study)
(bulged, conformation of, in soln., NMR study of)
IT **Conformation and Conformers**
(of bulged DNA, in soln., NMR study of)
IT Nuclear magnetic resonance
(of bulged deoxyribonucleotide, proton resonances assignment in)
IT Nucleic acid bases
RL: BIOL (Biological study)
(pairs, of bulged DNA, distortions in)
IT **Nucleotides, polymers**
RL: BIOL (Biological study)
(**oligo-**, **deoxyribo-**, bulged, double-stranded, soln. conformation of, NMR study of)
IT 147306-88-5 147306-89-6

RL: PRP (Properties)
(conformation of, in soln., NMR study of)
IT 1333-74-0
RL: PRP (Properties)
(nuclear magnetic resonance, of bulged deoxyribonucleotide, proton resonances assignment in)

=> d ibib abs ind 8

L33 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1992:168491 HCAPLUS
DOCUMENT NUMBER: 116:168491
TITLE: Chemistry of .alpha.-amino nitriles. 5. Why pentose and not hexose nucleic acids? Part I. Introduction to the problem, conformational analysis of oligonucleotide single strands containing 2',3'-dideoxyglucopyranosyl building blocks (homo-DNA), and reflections on the conformation of A- and **B-DNA**
AUTHOR(S): Eschenmoser, Albert; Dobler, Max
CORPORATE SOURCE: Org.-Chem. Lab., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.
SOURCE: Helv. Chim. Acta (1992), 75(1), 218-59
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Homo-DNA oligonucleotides were prepd. and paired, and structures and other properties were detd. Single-stranded backbone structure of 2',3'-dideoxyglucopyranose oligonucleotides predicted a linear conformation for the strand. This conformation occurs in **A-DNA** duplexes. Backbones of DNA single strands are predisposed to the helicity of A- or **B-DNA** duplexes. Helicity hinges primarily on the 5-membered sugar rings (pentoses).
CC 6-2 (General Biochemistry)
ST DNA conformation A B pentose
IT Deoxyribonucleic acids
RL: BIOL (Biological study)
(deoxyribose of, in A and B conformation, pentoses and hexoses in relation to)
IT **Conformation and Conformers**
(**A**, of DNA, deoxyribose in, pentoses and hexoses in relation to)
IT **Conformation and Conformers**
(**B**, of DNA, deoxyribose in, pentoses and hexoses in relation to)
IT **Nucleotides, polymers**
RL: BIOL (Biological study)
(oligo-, dideoxyglucopyranose-contg., pyranose in conformation of, pentoses and hexoses in relation to)
IT **Nucleotides, polymers**
RL: BIOL (Biological study)
(**oligo-**, **deoxyribo-**, deoxyribose of, conformation dependence on, pentoses and hexoses in relation to)
IT 140147-35-9
RL: PRP (Properties)
(of DNA analog, in A conformation, deoxyribose in relation to)
IT 533-67-5, Deoxyribose
RL: PRP (Properties)
(of DNA, in A and B conformations, dideoxyglucopyranose in relation to)

=> d ibib abs ind 9

L33 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1992:54988 HCAPLUS
DOCUMENT NUMBER: 116:54988
TITLE: Solution structure of [d(GTATATAC)]2 via restrained molecular dynamics simulations with nuclear magnetic resonance constraints derived from relaxation matrix analysis of two-dimensional nuclear Overhauser effect experiments
AUTHOR(S): Schmitz, Uli; Pearlman, David A.; James, Thomas L.
CORPORATE SOURCE: Dep. Pharm. Chem., Univ. California, San Francisco, CA, 94143-0446, USA
SOURCE: J. Mol. Biol. (1991), 221(1), 271-92
CODEN: JMOBAK; ISSN: 0022-2836
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two-dimensional nuclear Overhauser effect (2D NOE) spectra have been used as the exptl. basis for detg. the soln. structure of the duplex [d(GTATATAC)]2 employing restrained mol. dynamics (rMD) simulations. The MARDIGRAS algorithm has been employed to construct a set of 233 interproton distance constraints via iterative complete relaxation matrix anal. utilizing the peak intensities from the 2D NOE spectra obtained for different mixing times and model structures. The upper and lower bounds for each of the constraints, defining size of a flat-well potential function term used in the rMD simulations, were conservatively chosen as the largest or smallest value calcd. by MARDIGRAS. Three different starting models were utilized in several rMD calcns.: energy-minimized **A-DNA**, **B-DNA**, and a structure contg. wrinkled D-DNA in the interior. Considerable effort was made to define the appropriate force consts. to be employed with the NOE terms in the AMBER force field, using as criteria the av. constraints deviation, the constraints violation energy and the total energy. Of the 233 constraints, one was generated indirectly, but proved to be crucial in defining the structure: the cross-strand A5-H2 A5-H2 distance. As those two protons resonate isochronously for the self-complementary duplex, the distance cannot be detd. directly. However, the general pattern of 2D NOE peak intensities, spin-lattice relaxation time (T1) values, and 31P NMR spectra lead to use of the A3-H2 A7-H2 distance for A5-H2 A5-H2 as well. Five rMD runs, with different random no. seeds, were made for each of the starting structures with the full distance constraint set. The av. structure from all 15 runs and the five-structure avs. from each starting structure were all quite similar. Two rMD runs for each starting structure were made with the A5-H2 A5-H2 constraint missing. The av. of these six rMD runs revealed differences in structure, compared to that with the full set of constraints, primarily for the middle two base-pairs involving the missing cross-strand constraint but global deviations also were found. Conformational anal. of the resulting structures revealed that the inner four to six base-pairs differed in structure from the termini. Furthermore, an alternating structure was suggested with features alternating for the A-T and T-A steps.

CC 9-15 (Biochemical Methods)
Section cross-reference(s): 3, 6
ST oligonucleotide soln structure detn; mol dynamics simulation oligonucleotide; NMR spectrometry oligonucleotide; nuclear Overhauser effect oligonucleotide
IT Algorithm
(for oligonucleotide soln. structures detn., MARDIGRAS)
IT Mathematics

(for oligonucleotide structure detn.)
IT **Conformation and Conformers**
(soln., of oligonucleotides, detn. of)
IT **Conformation and Conformers**
(**A**, of DNA)
IT **Conformation and Conformers**
(**B**, of DNA)
IT **Conformation and Conformers**
(D, of DNA)
IT **Nucleotides, polymers**
RL: PRP (Properties)
(oligo-, soln. structures of, detn. of)
IT Overhauser effect
(two-dimensional, for oligonucleotide structure detn.)
IT 91605-96-8
RL: PRP (Properties)
(soln. structures of, detn. of)

=> d ibib abs ind 10

L33 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:628324 HCAPLUS
DOCUMENT NUMBER: 111:228324
TITLE: Determination of the DNA sugar pucker using carbon-13 NMR spectroscopy
AUTHOR(S): Santos, Rodolfo A.; Tang, Pei; Harbison, Gerard S.
CORPORATE SOURCE: Dep. Chem., State Univ. New York, Stony Brook, NY, 17794, USA
SOURCE: Biochemistry (1989), 28(24), 9372-8
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Solid-state 13C NMR spectroscopy of a series of cryst. nucleosides and nucleotides allows direct measurement of the effect of the deoxyribose ring conformation on the C chem. shift. The 3'-endo conformers have 3' and 5' chem. shifts significantly (5-10 ppm) upfield of comparable 3'-exo and 2'-endo conformers. The latter 2 conformers may be distinguished by smaller but still significant differences in the C chem. shifts at the C-2' and C-4' position. High-resoln. solid-state NMR of 3 modifications of fibrous calf thymus DNA shows that these trends are maintained in high-mol.-wt. DNA and confirms that the major ring pucker in **A-DNA** is 3'-endo, whereas both **B-DNA** and C-DNA are largely 2'-endo. Thus, 13C NMR spectroscopy is a striaghtforward and useful probe of DNA ring pucker in both soln. and the solid state.

CC 9-5 (Biochemical Methods)
Section cross-reference(s): 6, 33

ST DNA sugar pucker detn NMR; NMR spectrometry deoxyribose conformation detn; carbon 13 NMR DNA sugar

IT Nucleosides, properties
**Nucleotides, properties**
RL: PRP (Properties)
(carbon-13 NMR chem. shift of, deoxyribose pucker detn. in relation to)

IT Deoxyribonucleic acids
RL: ANST (Analytical study)
(deoxyribose of, conformational pucker detn. in, by carbon-13 NMR)

IT **Conformation and Conformers**
(of deoxyribose of DNA, pucker detn. in, by carbon-13 NMR)

IT Nuclear magnetic resonance
(of nucleosides and nucleotides)

IT 54-42-2, 5-Iodo-2'-deoxyuridine 59-14-3 611-53-0, 5-Iodo-2'-deoxycytidine 951-77-9, 2'-Deoxycytidine 958-09-8, 2'-Deoxyadenosine 1022-79-3, 5-Bromo-2'-deoxycytidine 1032-65-1, 2'-Deoxycytidine-5'-phosphate
RL: PRP (Properties)
(carbon-13 NMR chem. shift of, deoxyribose pucker detn. in relation to)

IT 533-67-5, Deoxyribose
RL: ANST (Analytical study)
(conformational pucker of, detn. of, in DNA by carbon-13 NMR)

=> d ibib abs ind 11

L33 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:511155 HCAPLUS
DOCUMENT NUMBER: 111:111155
TITLE: Characterization of the base stacking interactions in DNA by means of Lennard-Jones empirical potentials
AUTHOR(S): Sponer, J.; Kypr, J.
CORPORATE SOURCE: Fac. Nat. Sci., J. E. Purkinje Univ., Brno, 61137, Czech.
SOURCE: Gen. Physiol. Biophys. (1989), 8(3), 257-72
CODEN: GPBIE2; ISSN: 0231-5882
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Three empirical potentials of the Lennard-Jones type taken from literature were used to calc. van der Waals contributions to the base-pair couples stacking energies in **B-DNA** and **A-DNA** type double helical conformations. The information obtained can be summarized as follows. Purine-pyrimidine and purine-purine (pyrimidine-pyrimidine in the complementary strand) sequences preferred right-handed helical arrangement, whereas pyrimidine-purine sequences favored left-handed (C-G) or unwound (T-A) stacking geometry; in the latter case this only held for B- but not **A-DNA** (the C-G sequence was not studied in **A-DNA** owing to difficulties (see below) with the G amino group in G-DNA). Pos. propeller twist of base-pairs was stable in both B- and **A-DNA**; the thymine Me group promoted the propeller and this effect was strongest in the A-T step. Tilt of base pairs occurred around zero in **B-DNA** and between 13-20.degree. in **A-DNA**, in agreement with the exptl. observations. Vertical sepn. of base pairs was optimal within 0.33-0.34 nm for **B-DNA** and around 0.29 nm for **A-DNA** using the 9-6 potential. The 12-6 potential gave similar results with **B-DNA** as the 9-6 potential if, however, base pairs were sepd. by 0.35-3.36 nm. The calcd. effect of the guanine amino group was substantially stronger than expected on the basis of data derived from x-ray diffraction studies of oligonucleotide single crystals. In comparison with the 9/6 potential, the 12-6 potential provided more strict energy min. In summary, the empirical potentials reproduce, at least semiquant., many but not all DNA properties; this should be taken into account whenever the potentials are used for prediction purposes.
CC 6-2 (General Biochemistry)
ST DNA base stacking interaction potential
IT Deoxyribonucleic acids
RL: BIOL (Biological study)
(base stacking in, potential energy calcns. of)
IT Potential energy and function
(of DNA, base stacking interactions in relation to)
IT **Conformation and Conformers**
(of nucleic acids and DNA, base stacking effects on)
IT **Nucleotides, properties**
RL: BIOL (Biological study)
(deoxyribo-, base stacking in, potential energy calcns. of)
IT Force
(van der Waals, of DNA, base stacking interactions in relation to)
IT 1969-54-6, TpT 2764-25-2, DUpdU
RL: BIOL (Biological study)
(complex with deoxyadenylyldeoxyadenosine, base stacking interactions in)

IT 15180-30-0 122352-83-4, DIpdI
RL: BIOL (Biological study)
(complex with deoxycytidylyldeoxycytidine, base stacking interactions in)
IT 26467-01-6, DCpdC
RL: BIOL (Biological study)
(complex with deoxyguanylyldeoxyguanosine, and deoxyinosinylyldeoxyinosine, base stacking interactions in)
IT 23339-45-9
RL: BIOL (Biological study)
(complex with thymidylylthymidine and deoxyuridylyldeoxyuridine, base stacking interactions in)
IT 47792-43-8, DIpdC 122352-84-5, DCpdI???
RL: BIOL (Biological study)
(double-standed, base stacking interactions in)
IT 15178-66-2, DCpdG 19192-40-6, DTpdA 23339-47-1, DApdT 23405-83-6
69165-69-1, DUpdA 76619-73-3, DApdU
RL: BIOL (Biological study)
(double-stranded, base stacking interactions in)

=> d ibib abs ind 12

L33 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:436076 HCAPLUS
DOCUMENT NUMBER: 111:36076
TITLE: Analysis of the relative contributions of the nuclear Overhauser interproton distance restraints and the empirical energy function in the calculation of oligonucleotide structures using restrained molecular dynamics
AUTHOR(S): Gronenborn, Angela M.; Clore, G. Marius
CORPORATE SOURCE: Lab. Chem. Phys., Natl. Inst. Diabetes Dig. Kidney Disord., Bethesda, MD, 20892, USA
SOURCE: Biochemistry (1989), 28(14), 5978-84
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The relative contributions of the interproton distance restraints derived from nuclear Overhauser enhancement measurements and of the empirical energy function in the detn. of oligonucleotide structures by restrained mol. dynamics were investigated. The calcns. are based on 102 intraresidue and 126 interresidue interproton distance restraints derived from short mixing time 2-dimensional nuclear Overhauser enhancement data on the dodecamer 5'd(CGCGPATTCGCG)2 (Clore, G. M. et al., 1988). Eight interproton distance restraint lists were made up with errors ranging from -0.1/+0.2 to -1.2/+1.3 .ANG. for r < 2.5 .ANG. and from -0.2/+0.3 to -1.3/+1.4 .ANG. for r .gtoreq. 2.5 .ANG.. These restraints were incorporated into the total energy function of the system in the form of square-well potentials with force consts. set sufficiently high to ensure that the deviations between calcd. distances and exptl. restraints were very small (av. interproton distance root mean square deviation of <0.06 .ANG.). For each data set, 6 calcns. were done, 3 starting from classical **A-DNA** and 3 from classical **B-DNA**.
Apparently, structural changes occurring during the course of restrained mol. dynamics and the degree of structural convergence were detd. by the interproton distance restraints. All the structures display similar small deviations from idealized geometry and have the same values for the nonbonding energy terms comprising van der Waals, electrostatic, and H-bonding components. Thus, the function of the empirical energy function is to maintain near perfect stereochem. and nonbonded interactions. Local structural variations can be detd. up to error limits of -0.2/+0.3 .ANG. for r < 2.5 .ANG. and -0.3/+0.4 .ANG. for r .gtoreq. 2.5 .ANG.. Up to error limits of -0.4/+0.5 .ANG. for r < 2.5 .ANG. and -0.5/+0.6 .ANG. for r .gtoreq. 2.5 .ANG., local structural variations are still discernible, although the spread of the structures becomes appreciably larger. For larger error limits, local structural variations cannot be assessed at all.

CC 9-5 (Biochemical Methods)
Section cross-reference(s): 6, 33, 77

ST NOE oligonucleotide structure detn mol dynamics; Overhauser effect oligonucleotide structure detn; energy function oligonucleotide structure detn; oligonucleotide structure detn mol dynamics; conformation detn oligonucleotide

IT Chains, chemical
(dynamics of, of oligonucleotides, in structure detn., Overhauser enhancement in)

IT Overhauser effect
(in oligonucleotide structure calcn., interproton distance restraints contribution in relation to)

IT **Conformation and Conformers**
(of oligonucleotides, calcn. of, restrained mol. dynamics method in, nuclear Overhauser interproton distance restraints and empirical energy function contribution in)

IT Potential energy and function
(conformational, in oligonucleotide structure calcn., interproton distance restraints from NOE data in relation to)

IT **Nucleotides, polymers**
RL: PRP (Properties)
(oligo-, structure of, calcn. of, by restrained mol. dynamics method, nuclear Overhauser interproton distance restraints and empirical energy function contributions in)

IT 114155-95-2
RL: ANST (Analytical study)
(double-stranded, structure of, calcn. of, by restrained mol. dynamics method, nuclear Overhauser interproton distance restraints and empirical energy function contributions in)

=> d ibib abs ind 13

L33 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:402811 HCAPLUS
DOCUMENT NUMBER: 111:2811
TITLE: Sequence specificity in spermine-induced structural changes in CG-oligomers
AUTHOR(S): Majumder, Kumud; Brahmachari, Samir K.
CORPORATE SOURCE: Mol. Biophys. Unit, Indian Inst. Sci., Bangalore, 560 012, India
SOURCE: Biochem. Int. (1989), 18(2), 455-65
CODEN: BIINDF; ISSN: 0158-5231
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The role of spermine in inducing **A-DNA** conformation in deoxyoligonucleotides was studied using CCGG and GGCC as model sequences. Whereas CCGG adopts an alternating **B-DNA** conformation in low salt soln. at low temp., addn. of spermine to this medium induces a B .fwdarw. A transition. In contrast, the **A-DNA**-like structure of GGCC in low salt soln. at low temp. does not change under the influence of spermine. This suggests a sequence-dependent behavior of spermine. Further these results suggest that the **A-DNA** conformation obsd. in the crystals of d(ICCGG) and d(GGCC)2 might have been due to the presence of spermine in the crystn. cocktail.
CC 6-2 (General Biochemistry)
ST DNA conformation spermine sequence specificity; oligodeoxyribonucleotide conformation spermine sequence specificity
IT Deoxyribonucleic acids
RL: PRP (Properties)
(conformation of, spermine effect on, sequence specificity in)
IT **Conformation and Conformers**
(of oligodeoxyribonucleotides, spermine effect on, sequence specificity in)
IT **Nucleotides, polymers**
RL: PRP (Properties)
(**oligo-**, **deoxyribo-**, conformation of, spermine effect on, sequence specificity in)
IT 71-44-3, Spermine
RL: BIOL (Biological study)
(DNA conformation response to, sequence specificity in)
IT 64108-55-0 106867-95-2
RL: PRP (Properties)
(conformation of)
IT 64108-56-1
RL: PRP (Properties)
(conformation of, spermine effect on, sequence specificity in)

=> d ibib abs ind 14

L33 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1988:89788 HCAPLUS
DOCUMENT NUMBER: 108:89788
TITLE: The potentially Z-DNA-forming sequence d(GTGTACAC) crystallizes as **A-DNA**
AUTHOR(S): Jain, Sanjeev; Zon, Gerald; Sundaralingam, Muttaiya
CORPORATE SOURCE: Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA
SOURCE: J. Mol. Biol. (1987), 197(1), 141-5
CODEN: JMOBAK; ISSN: 0022-2836
DOCUMENT TYPE: Journal
LANGUAGE: English

AB (GT)n/(CA)n sequences frequently occur in eukaryotic DNA and have potential for forming left-handed Z-DNA. The x-ray crystal structure of a self-complementary octadeoxynucleotide, d(GTGTACAC), is reported at 2.5 .ANG. resoln. The mol adopts the right-handed double-helical conformation of **A-DNA**. In this alternating purine-pyrimidine DNA minihelix, the roll and twist angles show alternations qual. consistent with Calladine's rules. The av. tilt angle of 9.3.degree. is between the values found in **A-DNA** (19.degree.) and **B-DNA** (-6.degree.) fibers. Such intermediate conformations may render diversity to genomic DNA. The base-pair tilt angles and base-pair displacements from the helix axis are correlated for the known **A-DNA** double-helical fragments.

CC 6-2 (General Biochemistry)
Section cross-reference(s): 75

ST deoxynucleotide crystal structure **A DNA**; purine pyrimidine alternating DNA crystal structure

IT Deoxyribonucleic acids
RL: BIOL (Biological study)
(conformation of purine-pyrimidine-alternating)

IT **Crystal structure**
(of purine-pyrimidine-alternating octadeoxynucleotide **A-DNA** form)

IT **Conformation and Conformers**
(**A**, of self-complementary purine-pyrimidine-alternating octadeoxynucleotide)

IT **Nucleotides, polymers**
RL: BIOL (Biological study)
(**oligo-**, **deoxyribo-**, purine-pyrimidine-alternating, conformation of)

IT 113023-70-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and detritylation of double-stranded)

IT 113023-69-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of double-stranded, and A conformation)

=> d ibib abs ind 15

L33 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:221630 HCAPLUS
DOCUMENT NUMBER: 104:221630
TITLE: Structure refinement of oligonucleotides by molecular dynamics with nuclear Overhauser effect interproton distance restraints: application to 5' d(C-G-T-A-C-G)2
AUTHOR(S): Nilsson, Lennart; Clore, G. Marius; Gronenborn, Angela M.; Brunger, Axel T.; Karplus, Martin
CORPORATE SOURCE: Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA
SOURCE: J. Mol. Biol. (1986), 188(3), 455-75
CODEN: JMOBAK; ISSN: 0022-2836
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The soln. structure of the self-cDNA hexamer 5' d(C-G-T-A-C-G)2 is refined by restrained mol. dynamics in which 192 interproton distances, detd. from pre-steady-state nuclear Overhauser enhancement measurements, are incorporated into the total energy of the system in the form of effective potentials. First the method is tested by applying an idealized set of distance restraints taken from classical **B-DNA** to a simulation starting off from **A-DNA** and vice versa. In both cases the expected transition between A- and **B-DNA** occurs. Second, a set of restrained mol. dynamics calcns. is done starting from both A- and **B-DNA** with the exptl. interproton distances for 5' d(C-G-T-A-C-G)2 as restraints. Convergence to the same B-type structure is achieved with the interproton distances equal to the measured values within exptl. error. The root-mean-square at. difference between the 2 av. restrained dynamics structures (<1 .ANG.) is approx. the same as the root-mean-square fluctuations of the atoms.

CC 9-10 (Biochemical Methods)
Section cross-reference(s): 6, 33
ST oligonucleotide mol dynamics nuclear Overhauser; DNA conformation mol dynamics
IT Deoxyribonucleic acids
RL: PRP (Properties)
(conformation of, mol. dynamics with nuclear Overhauser effect interproton distance restraints in study of)
IT Overhauser effect
(interproton distance restraints, mol. dynamics with, structure refinement of oligonucleotides by)
IT **Conformation and Conformers**
(of DNA, mol. dynamics with nuclear Overhauser effect interproton distance restraints in study of)
IT Process simulation, biological
(mol. dynamics, structure refinement of oligonucleotides by, with nuclear Overhauser effect interproton distance restraints)
IT **Nucleotides, properties**
RL: PRP (Properties)
(oligo-, structure of, refinement of, by mol. dynamics with nuclear Overhauser effect interproton distance restraints)
IT 77064-59-6
RL: ANST (Analytical study)
(double-stranded, structure refinement of, by mol. dynamics with nuclear Overhauser effect interproton distance restraints)

=> d ibib abs ind 16

L33 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1984:485860 HCAPLUS
DOCUMENT NUMBER: 101:85860
TITLE: Poly(8-bromodeoxyadenylic acid): properties of the polymer and contrast with the ribopolynucleotide analog
AUTHOR(S): Kanaya, Eiko Nakagawa; Howard, Frank B.; Frazier, Joe; Miles, H. Todd
CORPORATE SOURCE: Lab. Mol. Biol., Natl. Inst. Arthritis, Diabetes Dig. Kidney Dis., Bethesda, MD, 20205, USA
SOURCE: Biochemistry (1984), 23(18), 4219-25
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The introduction of the bulky 8-bromo substituent into adenine residues of polynucleotides has strikingly different consequences in the deoxyribo- and the ribopolynucleotide series. In earlier studies, poly(8-bromoadenylate) [(r8BrA)n] was found to form a very stable double-helical structure, but not to undergo interaction with potentially complementary polynucleotides. It is reported here that poly(8-bromodeoxyadenylate) [(d8BrA)n], in contrast to (r8BrA)n, does not form an ordered self-structure in 0.1M Na+, but appears to exist as an electrostatically expanded rigid rod with unusual CD properties at very low ionic strength. The deoxyribo polymer, moreover, readily forms double helixes with either deoxy- or ribopyrimidine polynucleotides, as studied by UV, CD, and IR spectroscopy. These complexes are destabilized, relative to those formed by poly(dA), possibly because energy is needed to convert the purine residues from a more stable syn to an anti conformation, required for heteroduplex formation. The CD spectrum of (d8BrA)n.cntdot.(dT)n is similar to that of **B DNA**. The deoxyribo-ribo hybrids, (d8BrA)n.cntdot.(rU)n and (d8BrA)n.cntdot.(rBrU)n, have CD spectra resembling those of **A DNA** or RNA. Unlike other deoxyribo-deoxyribo pairs, (d8BrA)n.cntdot.(dBrU)n however, has a CD spectrum resembling RNA and other A-form helixes.

CC 6-2 (General Biochemistry)
Section cross-reference(s): 33, 73
ST bromodeoxyadenylate polymer conformation property; polybromodeoxyadenylate conformation property
IT Ionic strength
(conformation of poly(bromodeoxyadenylate)-pyrimidine polynucleotide complexes response to)
IT Circular dichroism
Infrared spectra
Ultraviolet and visible spectra
(of poly(bromodeoxyadenylate)-pyrimidine polynucleotide complexes)
IT **Conformation and Conformers**
(of poly(bromodeoxyadenylate)-pyrimidine polynucleotide complexes, electronic spectra in relation to)
IT **Nucleotides, compounds**
RL: BIOL (Biological study)
(poly-, pyrimidine, poly(bromodeoxyadenylate) complexes, conformation of, electronic spectra in relation to)
IT 90968-89-1 90968-90-4 90968-91-5 90968-93-7 90968-95-9
RL: PRP (Properties)
(conformation of, electronic spectra in relation to)
IT 14985-44-5

RL: PRP (Properties)
(polymn. and UV spectra of)

=> d ibib abs ind 17

L33 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1983:501075 HCAPLUS
DOCUMENT NUMBER: 99:101075
TITLE: Helix geometry and hydration in **A-DNA**, **B-DNA**, and Z-DNA
AUTHOR(S): Dickerson, R. E.; Drew, Horace R.; Conner, B. N.; Kopka, M. L.; Pjura, P. E.
CORPORATE SOURCE: Mol. Biol. Inst., Univ. California, Los Angeles, CA, 90024, USA
SOURCE: Cold Spring Harbor Symp. Quant. Biol. (1983), Volume Date 1982, 47(1), 13-24
CODEN: CSHSAZ; ISSN: 0091-7451
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Crystal structure and conformational properties of the title DNAs, esp. the A- and B-forms, and their oligodeoxynucleotide models were discussed and related to their hydration chem. Although the tetrameric and octameric A-form nucleotide models are nearly isomorphous, the conformation of the sugar moieties in both A- and B-form models differ considerably with increasing chain length. Consideration of the helix geometry of the models indicated that the ordered hydration of the minor groove in **B-DNA**, which is not present in **A-DNA**, can be explained in structural terms, e.g., the narrowing of the minor groove in A-T-rich regions results from a greater propeller twist of A-T than G-C pairs and a reorientation of O and N hydration sites in a manner to optimize and stabilize bound water. In **A-DNA**, the minor groove is essentially unhydrated, whereas solvent ordering is obsd. in the major groove. In this DNA form, hydration is apparently a result of surface site availability and the tendency of water to adopt a lattice arrangement.

CC 6-2 (General Biochemistry)
ST helix geometry DNA hydration; conformation DNA oligodeoxynucleotide hydration; crystal structure DNA oligodeoxynucleotide hydration; oligodeoxynucleotide crystal structure hydration
IT Hydration, chemical
(of DNA A and B forms and oligodeoxyribonucleotides)
IT **Crystal structure**
(of DNA and oligodeoxyribonucleotides, hydration effect on)
IT **Conformation and Conformers**
(of DNA and oligodeoxyribonucleotides, hydration in relation to)
IT Deoxyribonucleic acids
RL: BIOL (Biological study)
(structure and hydration of A and B and Z forms of)
IT **Nucleotides, properties**
RL: PRP (Properties)
(oligodeoxyribo-, crystal structure and hydration of, as DNA models)
IT 77889-82-8
RL: PRP (Properties)
(crystal structure of, hydration in relation to)

=> d ibib abs ind 18

L33 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1983:84999 HCAPLUS
DOCUMENT NUMBER: 98:84999
TITLE: Flexibility of nucleic acid conformations. 1. Comparison of the intensities of the Raman-active backbone vibrations in double-helical nucleic acids and model double-helical dinucleotide crystals
AUTHOR(S): Thomas, Gerald A.; Peticolas, Warner L.
CORPORATE SOURCE: Inst. Mol. Biol., Univ. Oregon, Eugene, OR, 97403, USA
SOURCE: J. Am. Chem. Soc. (1983), 105(4), 986-92
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Raman spectroscopic measurements were made on crystals of 3 dinucleotides, UpA, GpC, and pTpT, whose sugar-phosphate conformations are precisely known from x-ray diffraction measurements. UpA and GpC belong to the A-genus conformation with a C3-endo ribose ring pucker and exhibit the typical frequency and intensity of the A-genus Raman marker band. On the other hand, pTpT belongs to the B-genus (C2'-endo furanose ring conformation). For this latter crystal, the conformationally dependent B-genus Raman marker band at 833 cm-1 is much more intense than that found in ordinary **B-DNA** in fibers or in solns. These results are discussed with ref. to recent potential energy calcns. It is suggested that the deoxyribose rings in **B-DNA** are less rigid than in either **A-DNA** or ordered RNA. Some flexibility of the furanose rings is suggested to be responsible for the complete absence of either C2'- or C3'-endo marker bands for the dinucleotides in soln. at room temp.

CC 6-2 (General Biochemistry)
ST nucleotide dimer conformation Raman; dinucleotide conformation Raman
IT Deoxyribonucleic acids
RL: PRP (Properties)
(Raman spectra of, conformation in relation to)
IT Raman spectra
(of dinucleotides)
IT **Conformation and Conformers**
(of dinucleotides, Raman spectra in relation to)
IT **Nucleotides, properties**
RL: PRP (Properties)
(**di**-, Raman spectra of, conformation in relation to)
IT 3256-24-4 58002-80-5 61442-57-7
RL: PRP (Properties)
(Raman spectra of, conformation in relation to)

=> d ibib abs ind 19

L33 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1982:487240 HCAPLUS
DOCUMENT NUMBER: 97:87240
TITLE: Molecular structure of the octamer d(G-G-C-C-G-G-C-C): modified **A-DNA**
AUTHOR(S): Wang, Andrew H. J.; Fujii, Satoshi; Van Boom, Jacques H.; Rich, Alexander
CORPORATE SOURCE: Dep. Biol., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
SOURCE: Proc. Natl. Acad. Sci. U. S. A. (1982), 79(13), 3968-72
CODEN: PNASA6; ISSN: 0027-8424
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The deoxyribonucleotide fragment, d(G-G-C-C-G-G-C-C), was synthesized and crystd. and its 3-dimensional structure was detd. by x-ray diffraction techniques to a resoln. of 2.25 .ANG.. The mol. formed a right-handed double helix in which the 2 base pairs at either end of the mol. were in the conventional **A-DNA** conformation, whereas the central 4 base pairs had a modified form in which alternate residues had sugar conformations that were closer to those in **B-DNA** than in **A-DNA**. The mols. had an intermol. contact in which the planar terminal guanine-cytosine base pair lies on the flat minor groove surface of the **A-DNA** helix.

CC 6-2 (General Biochemistry)
Section cross-reference(s): 75
ST deoxyribonucleotide octamer crystal structure; DNA fragment crystal structure conformation
IT Deoxyribonucleic acids
RL: BIOL (Biological study)
(A-, crystal structure and conformation of models of)
IT **Nucleotides, properties**
RL: PRP (Properties)
(conformation and crystal structure of)
IT **Conformation and Conformers**
(of DNA-**A** model octadeoxyribonucleotides)
IT **Crystal structure**
(of d(G-G-C-C-G-G-C-C) and d(C-C-C-C-G-G-G-G))
IT 82695-55-4P 82709-23-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of, **A-DNA** conformation in relation to)

=> d ibib abs ind 20

L33 ANSWER 20 OF 20 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1978:165620 HCAPLUS
DOCUMENT NUMBER: 88:165620
TITLE: Conformational characteristics of dApdA, dApdT, dTpdA, and dTpdT from energy minimization studies
AUTHOR(S): Thiyagarajan, P.; Ponnuswamy, P. K.
CORPORATE SOURCE: Dep. Phys., Auton. Postgrad. Cent., Tiruchirapalli, India
SOURCE: Biopolymers (1978), 17(3), 533-53
CODEN: BIPMAA; ISSN: 0006-3525
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The conformational characteristics of the deoxydinucleoside monophosphates dApdA, dApdT, dTpdA, and dTpdT were studied using an improved set of energy parameters to calc. the total potential energy and an improved version of the minimization technique to minimize the total energy by allowing all 7 dihedral angles of the mol. fragment to vary simultaneously. The most preferred conformation in all these units usually corresponded to 1 of the 4 helical conformations, namely, the **A-DNA, B-DNA**, C-DNA, and Watson-Crick DNA models. These helical conformations differed in energies by .apprx.3 kcal/mol with respect to one another. The conformations which could promote a loop or bend in the backbone were, in general, less stable by .apprx. 3.5 kcal/mol with respect to the resp. lowest-energy helical conformation. There is apparently a definite influence of bases and their actual sequences on the preferred conformations of deoxydinucleoside monophosphates. The lowest-energy structure, although corresponding to 1 of the 4 helical conformations, differed with the type of deoxydinucleoside monophosphate. Base stacking was noted in dApdA and dTpdA with both C(3')-endo and C(2')-endo sugars and in dApdT and dTpdT with only C(3')-endo sugar. The inversion of the base sequence in deoxydinucleoside monophosphates altered the order of preference of low-energy conformations as well as the base-stacking property of the unit. Paths linking the starting and final states in the (.omega.',.omega.) plane showed interesting features with regard to the energy spread, thus providing insight into the path of conformational movement of the mol. under slight perturbation. The stabilities of the A and B forms, including the internal energies of the C(3')-endo and C(2')-endo sugar systems, indicated that for dTpdT the B .fwdarw. A transition is less probable. For dApdA, dApdT, and dTpdA this transition is probable in the same order of preference. The T-A sequence in the polynucleotide chain may serve as the site accessible for B .dblarw. A transitions.

CC 6-2 (General Biochemistry)
ST dinucleotide conformation; nucleotide di conformation; adenine thymine dinucleotide conformation
IT Bond angle
Bond length
(in deoxydinucleotides)
IT **Conformation and Conformers**
Potential energy and function
(of deoxydinucleotides)
IT Potential energy and function
(conformational, of deoxydinucleotides)
IT **Nucleotides, properties**
RL: PRP (Properties)
(deoxydi-, conformation and energy of)

IT 1969-54-6 19192-40-6 23339-45-9 23339-47-1
RL: PRP (Properties)
(conformation and energy of)

STR Search

KRISHNAN 09/970,971

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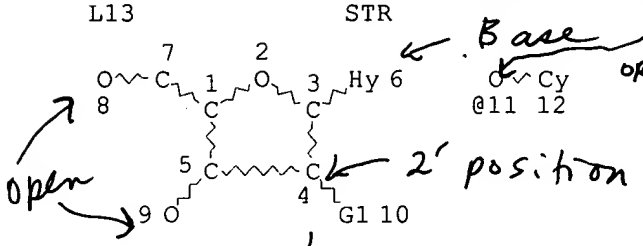
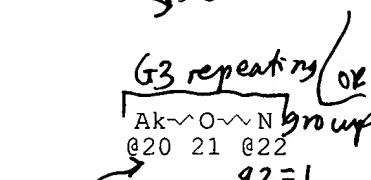



Cy = cyclic any kind

AK = alkyl, linear saturated ie. $-(CH_2)_n-$

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DEFAULT ECLEVEL IS LIMITED
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GRAPH ATTRIBUTES:
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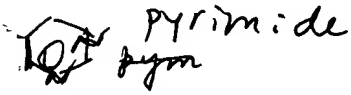


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L35             5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L31 AND L21
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L39             2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L38 NOT L12
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purine

must have phosphorus

must be in citation

2 citations

=> d ibib abs hitstr 1

L39 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:436086 HCAPLUS
DOCUMENT NUMBER: 121:36086
TITLE: Solution conformation of hexameric and heptameric lariat-RNAs and their self-cleavage reactions which give products mimicking those from some catalytic RNAs (ribozymes)
AUTHOR(S): Rousse, B.; Puri, N.; Viswanadham, G.; Agback, P.; Glemarec, C.; Sandstroem, A.; Sund, C.; Chattopadhyaya, J.
CORPORATE SOURCE: Biomed. Cent., Univ. Uppsala, Uppsala, S-751 23, Swed.
SOURCE: Tetrahedron (1994), 50(6), 1777-810
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English

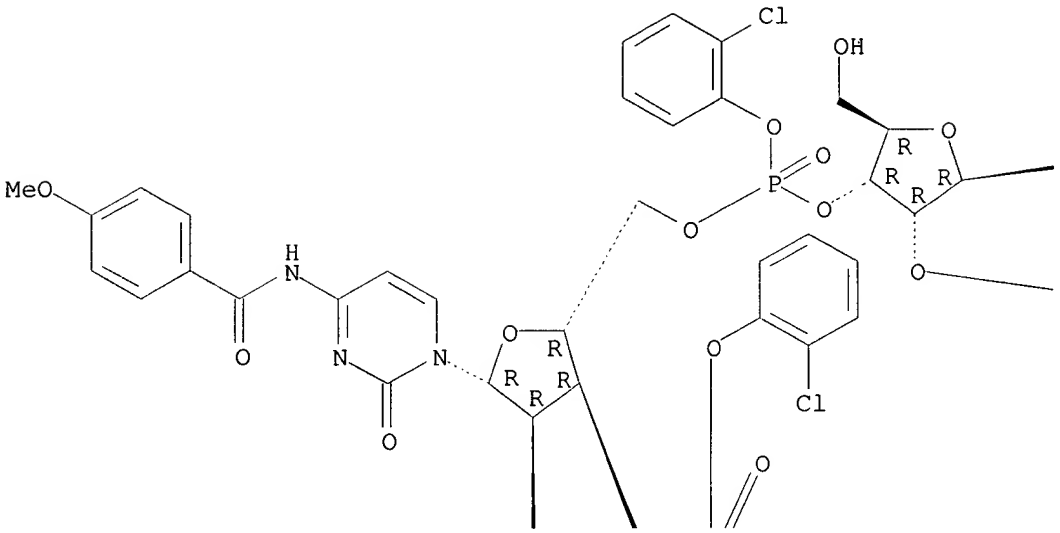
AB Small "lariat" hexameric and heptameric RNAs undergo self-cleavage, whereas the two cyclic A(2'-.fwdarw.5')G and A(3'.fwdarw.5')G linked tetramers do not self-cleave. The site of phosphodiester cleavage is specific and occurs at the 3'-phosphate of the guanosine residue to give a guanosine 2', 3'-cyclic phosphate and a 5'-hydroxyl termini. The rate of cleavage is temp. and pH dependent. The addn. of Mg2+ ions slightly increased the rate of cleavage, but NMR studies show that it does not produce any changes in the conformation of the ribose rings and of glycosidic bonds. 1H-NMR shows that the lariat-hexamer exists as two conformers (A and B) in slow exchange on the NMR time scale. The loop nucleotides in the **B-form** of the hexamer have ribose, glycoside bonds and phosphate backbone conformation. Torsonal constraints derived form 1H-1H, 1H-31P and 13C-31P coupling consts. were used for mol. dynamics simulations in water with sodium counterions for a total of 226 ps. The pH-dependent study of the self-cleavage reaction of the hexamer has shown that the self-cleavage rated peaks at pH 6 and slows down considerably both above and below this pH.

IT **154976-73-5P 154976-75-7P 154976-77-9P**
**154976-78-0P 154976-80-4P 154976-82-6P**
**154976-84-8P 154976-85-9P 154976-86-0P**
**154988-37-1P 154988-39-3P 154988-40-6P**
**155023-05-5P 155065-19-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in synthesis of oligoribonucleotides lariat RNAs)

RN 154976-73-5 HCAPLUS
CN 2'-Adenylic acid, P-(2-chlorophenyl)-N-[4-(1,1-dimethylethyl)benzoyl]-6-O-(2-nitrophenyl)-2'-O-(tetrahydro-2H-pyran-2-yl)guanylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-3-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-3'-O-[3-hydroxy-1,1,3,3-tetrakis(1-methylethyl)disiloxanyl]-N-(4-methoxybenzoyl)-, 2-chlorophenyl 2-cyanoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

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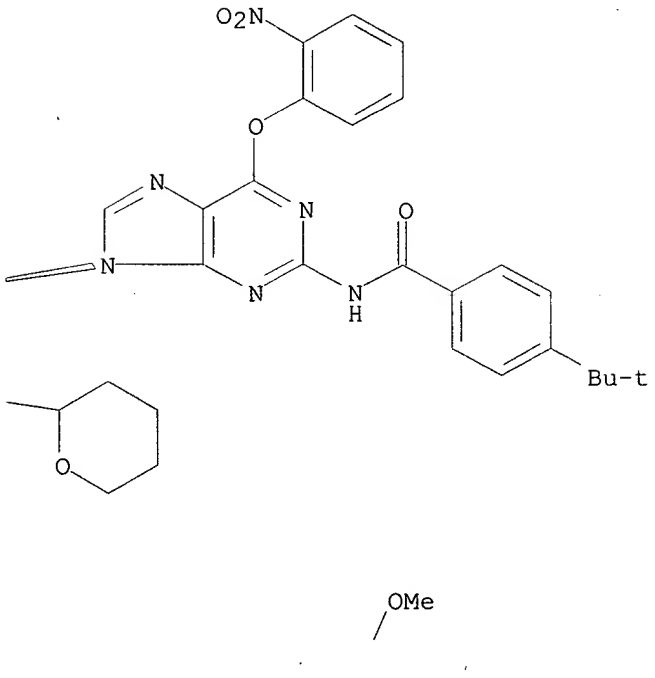

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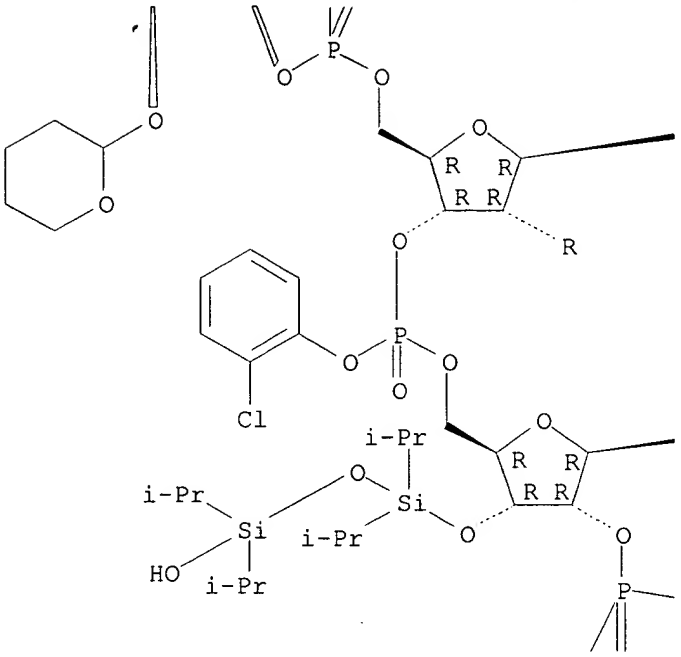


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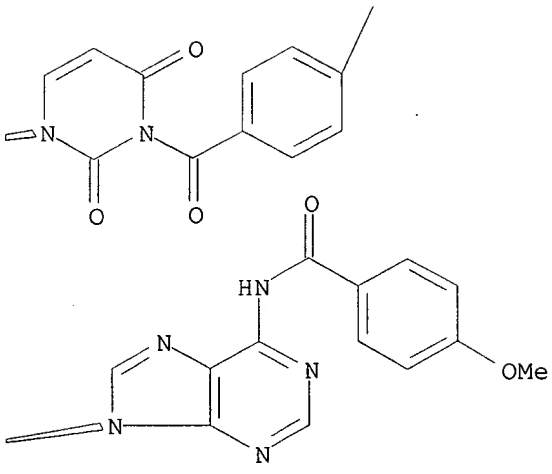


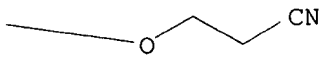

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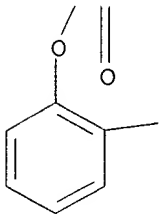

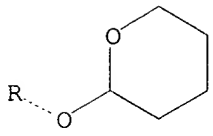

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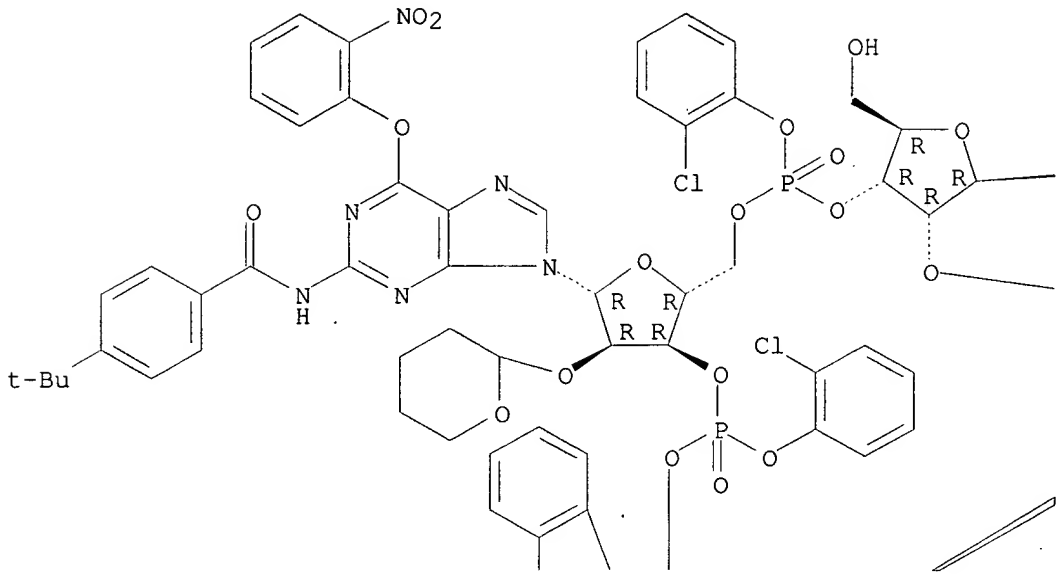
RN 154976-75-7 HCAPLUS
CN 3'-Uridylic acid, P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)adenylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-N-[4-(1,1-dimethylethyl)benzoyl]-6-O-(2-nitrophenyl)-2'-O-(tetrahydro-2H-pyran-2-yl)guanylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-3-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)-, 2-chlorophenyl 2-cyanoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

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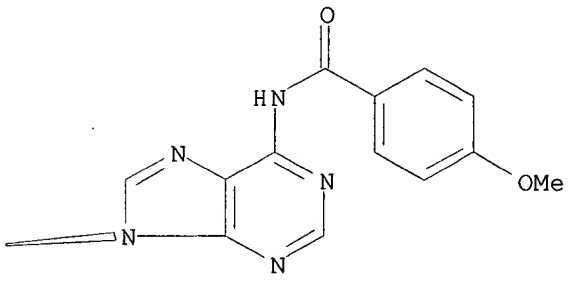


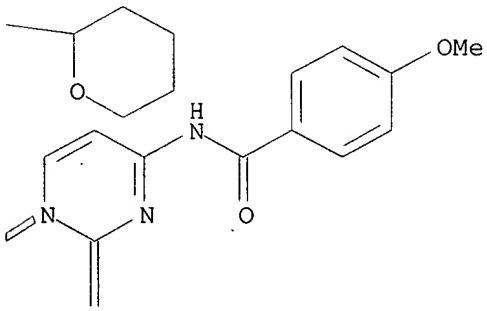

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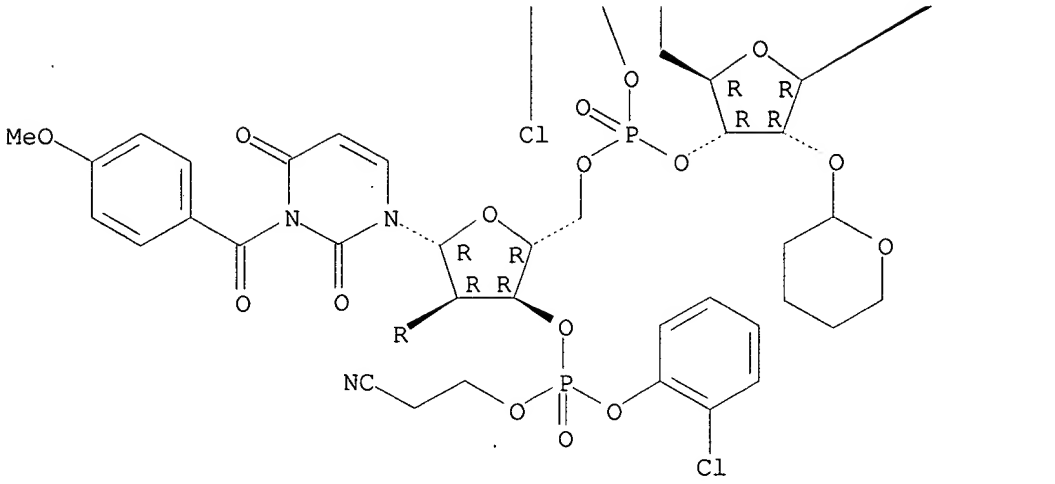

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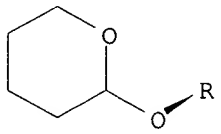
PAGE 3-A



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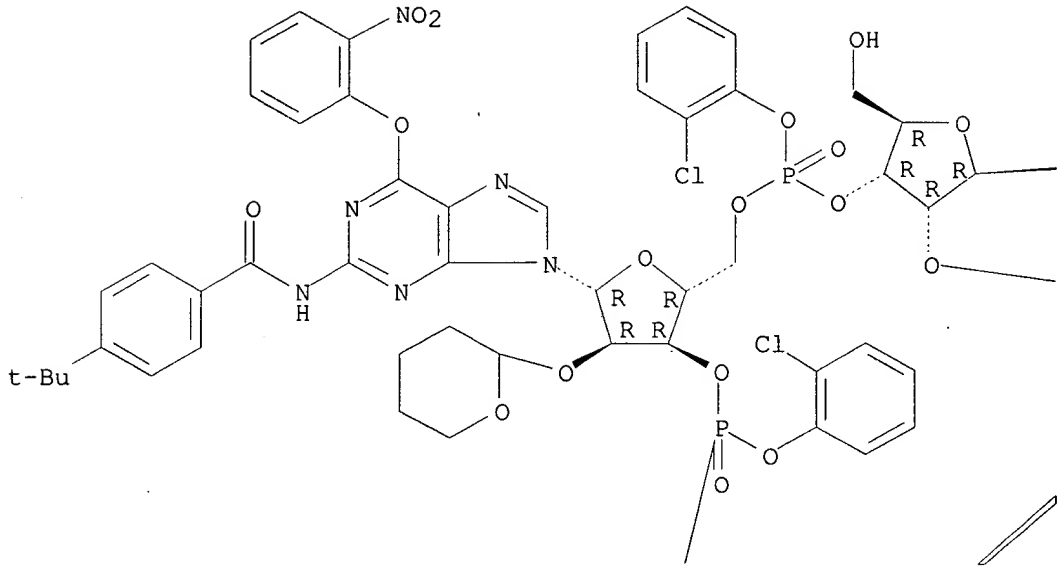
CN 3'-Uridylic acid, P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)adenylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-N-[4-(1,1-dimethylethyl)benzoyl]-6-O-(2-nitrophenyl)-2'-O-(tetrahydro-2H-pyran-2-yl)guanylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-3-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)-, mono(2-chlorophenyl) ester, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 154976-76-8
CMF C123 H126 Cl4 N16 O42 P4
CDES 5:ALL,B-D-RIBO

Absolute stereochemistry.

PAGE 1-A

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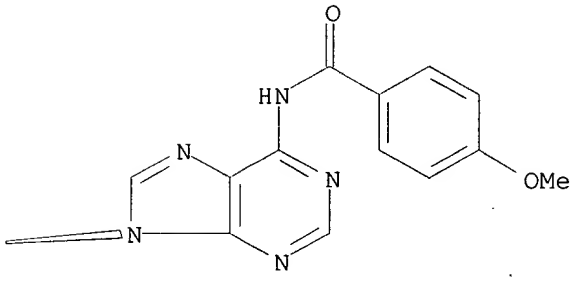


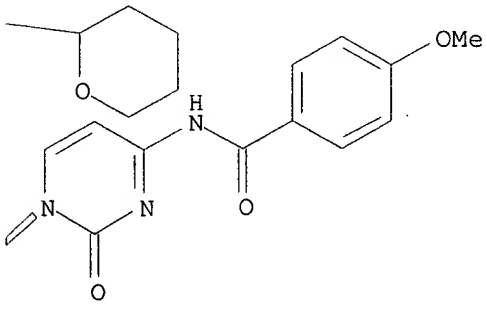

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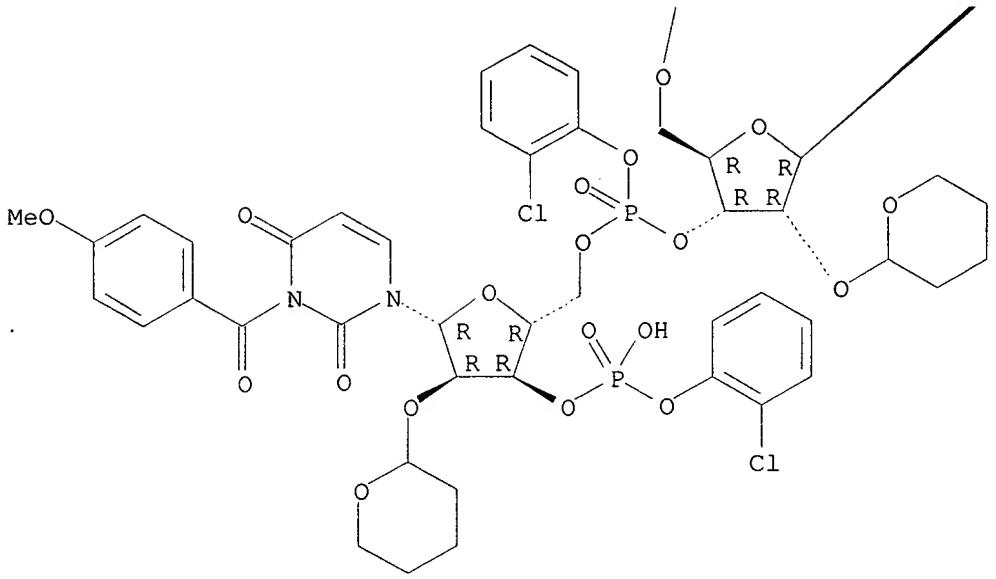

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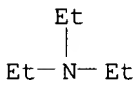
CMF C6 H15 N



RN 154976-78-0 HCAPLUS
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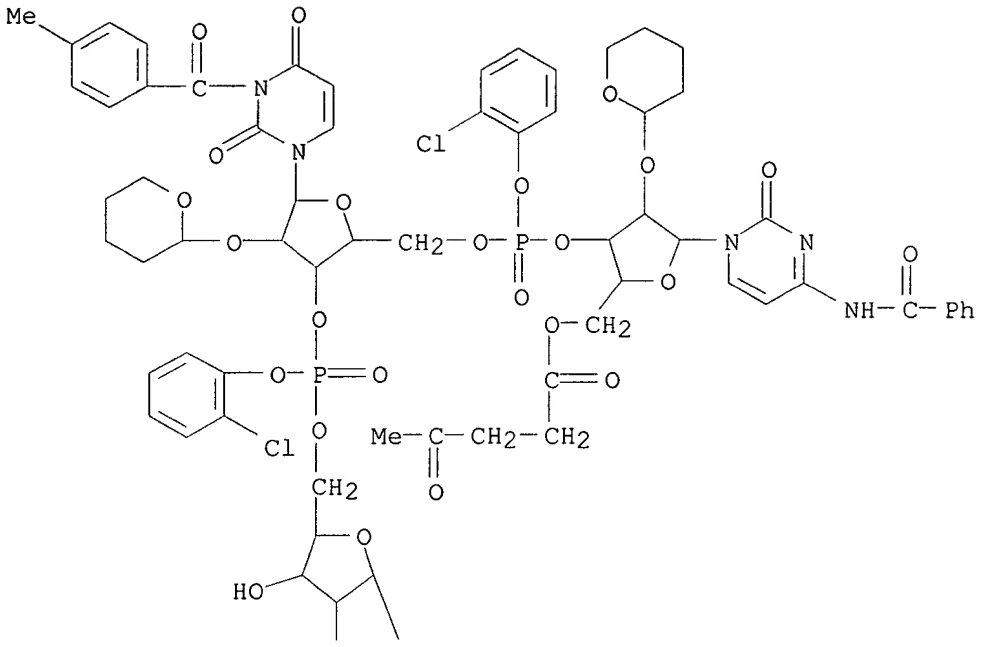
PAGE 1-A



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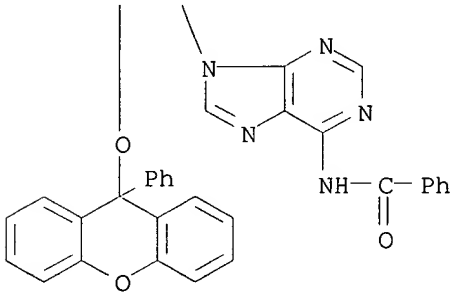

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CRN 154976-79-1
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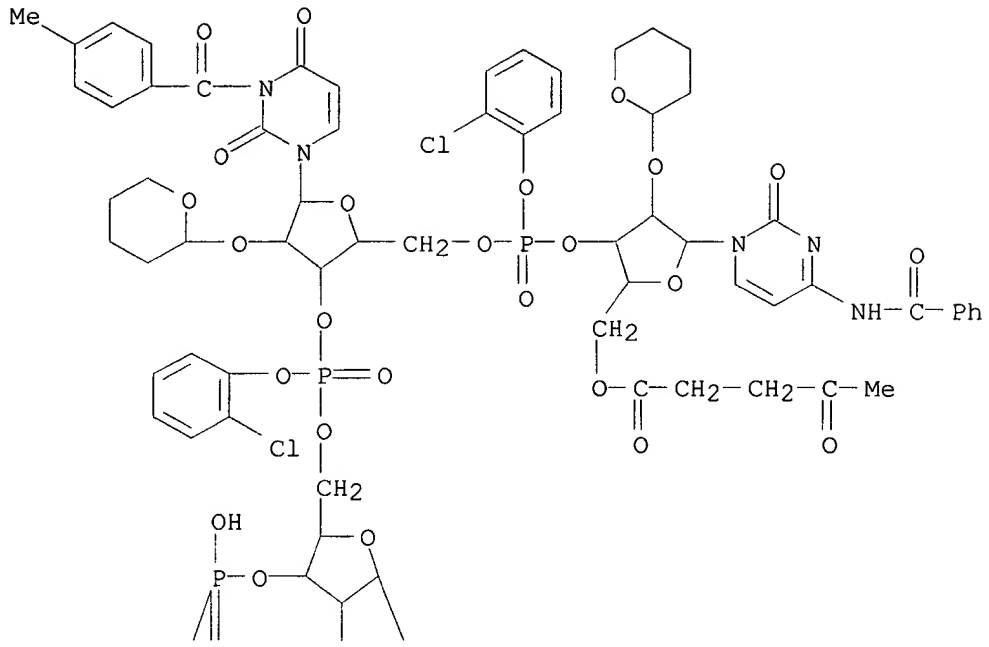
CDES 5:B-D-RIBO,B-D-RIBO,B-D-RIBO

PAGE 1-A



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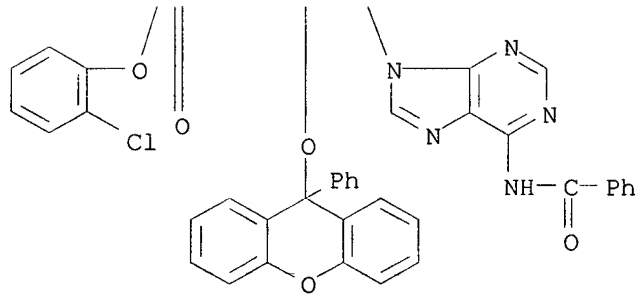

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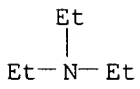

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methylbenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-N-benzoyl-, mono(2-chlorophenyl) ester, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 154976-81-5
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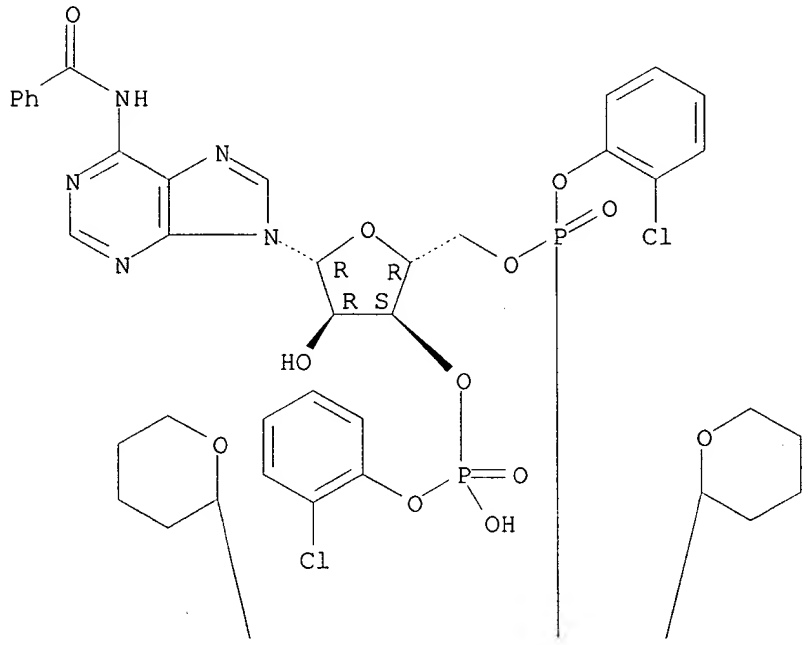
CDES 5:B-D-RIBO,B-D-RIBO,B-D-RIBO

Absolute stereochemistry.

PAGE 1-A



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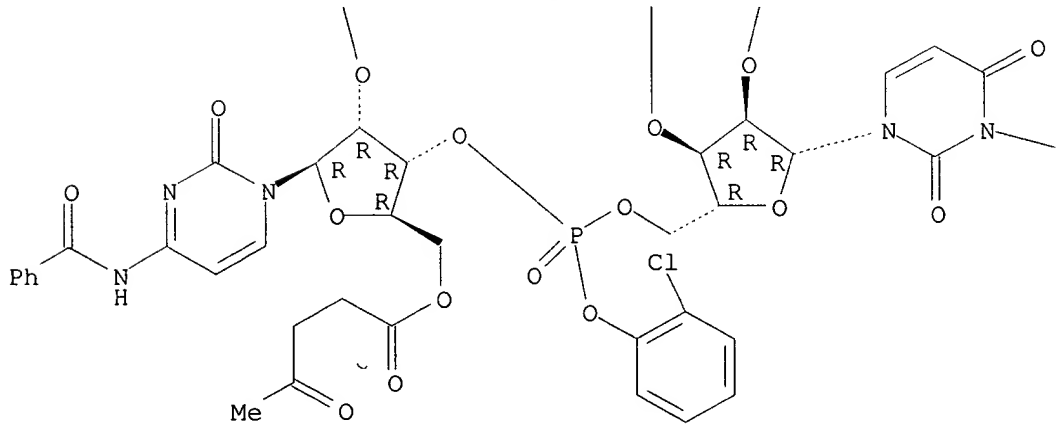

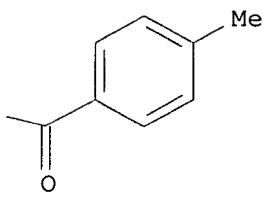


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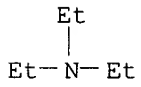


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CM 1

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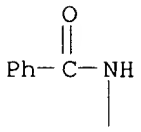
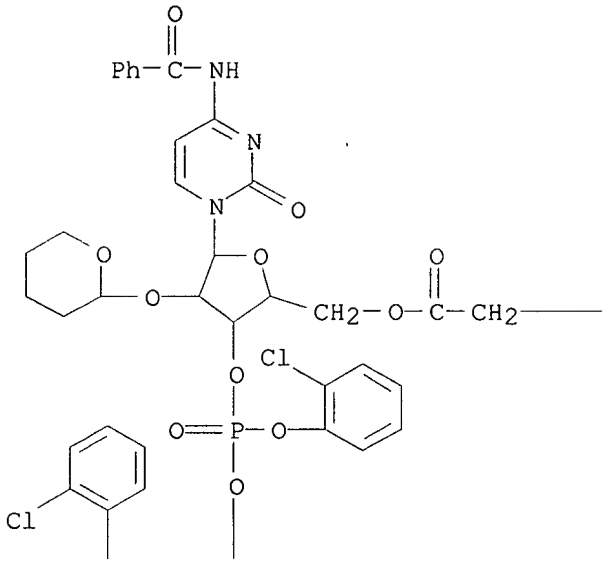
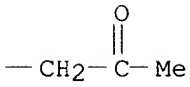
CDES 5:B-D-RIBO,B-D-RIBO,B-D-RIBO

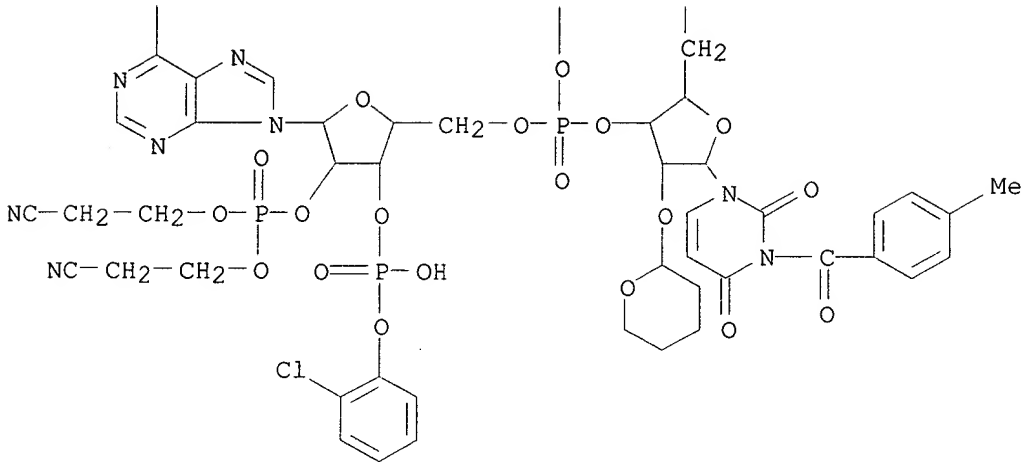
PAGE 1-A





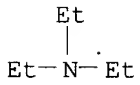
PAGE 1-B





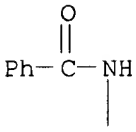
CM 2

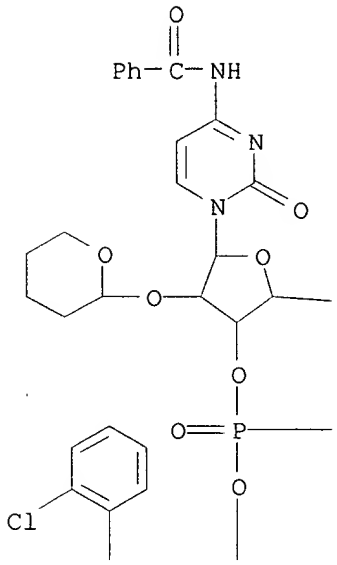
CRN 121-44-8
CMF C6 H15 N



RN 154976-85-9 HCAPLUS
CN Cytidine, N-benzoyl-P-(2-chlorophenyl)-5'-O-(1,4-dioxopentyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-3-(4-methylbenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-N-benzoyl-2'-O-[bis(2-cyanoethoxy)phosphinyl]-P-(2-chlorophenyl)adenylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-3-(4-methylbenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-N-benzoyl-, 2',3'-diacetate (9CI) (CA INDEX NAME)

PAGE 1-A





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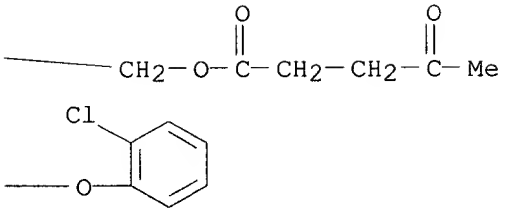

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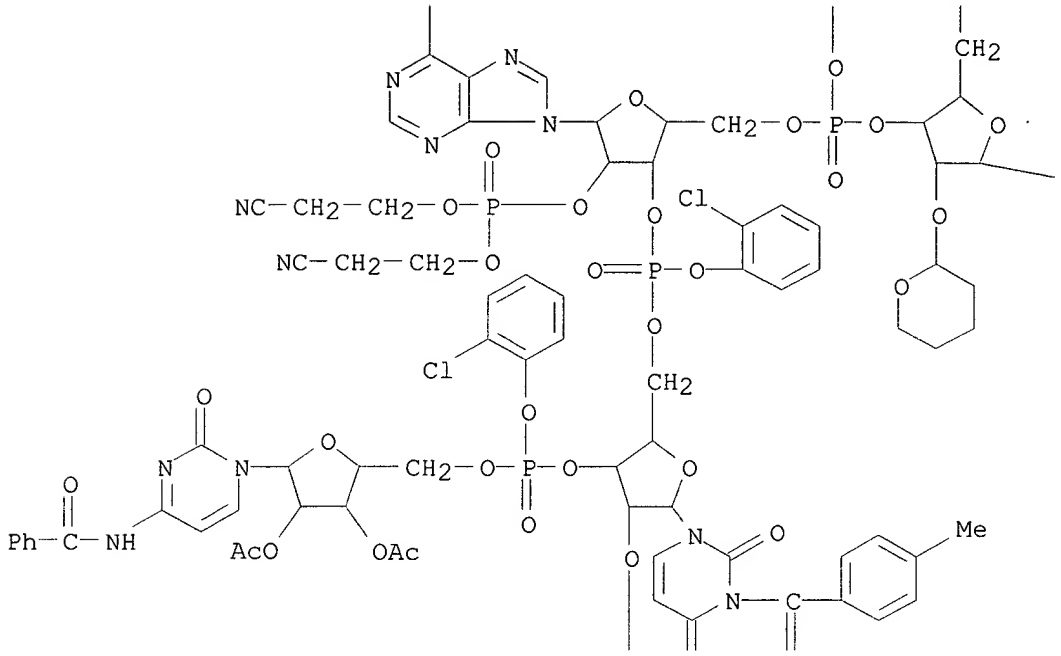
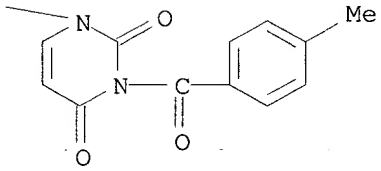
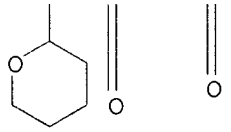


PAGE 2-B



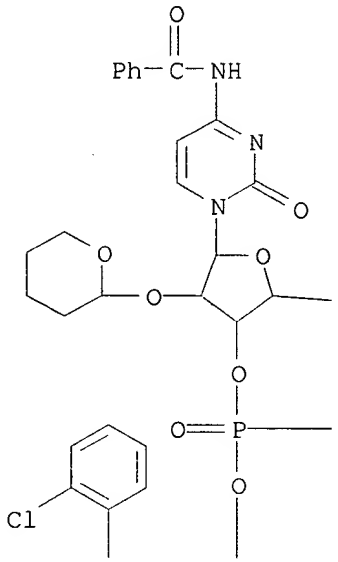
PAGE 3-A



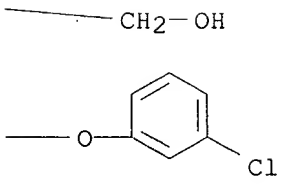
RN 154976-86-0 HCAPLUS
CN Cytidine, N-benzoyl-P-(2-chlorophenyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-3-(4-methylbenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-N-benzoyl-2'-O-[bis(2-cyanoethoxy)phosphinyl]-P-(2-chlorophenyl)adenylyl-(3'.fwdarw.5')-P-(2-

chlorophenyl)-3-(4-methylbenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-N-benzoyl-, 2',3'-diacetate (9CI) (CA INDEX NAME)

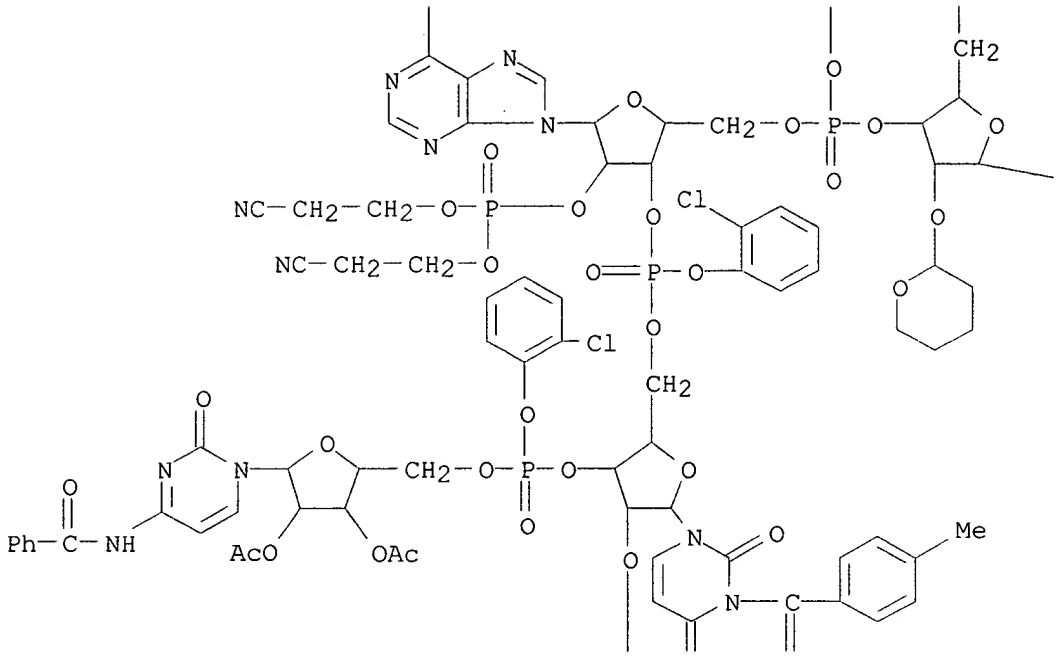
PAGE 1-A



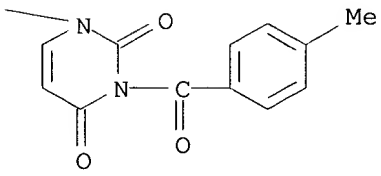
PAGE 1-B



PAGE 2-A



PAGE 2-B



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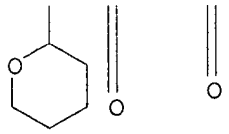
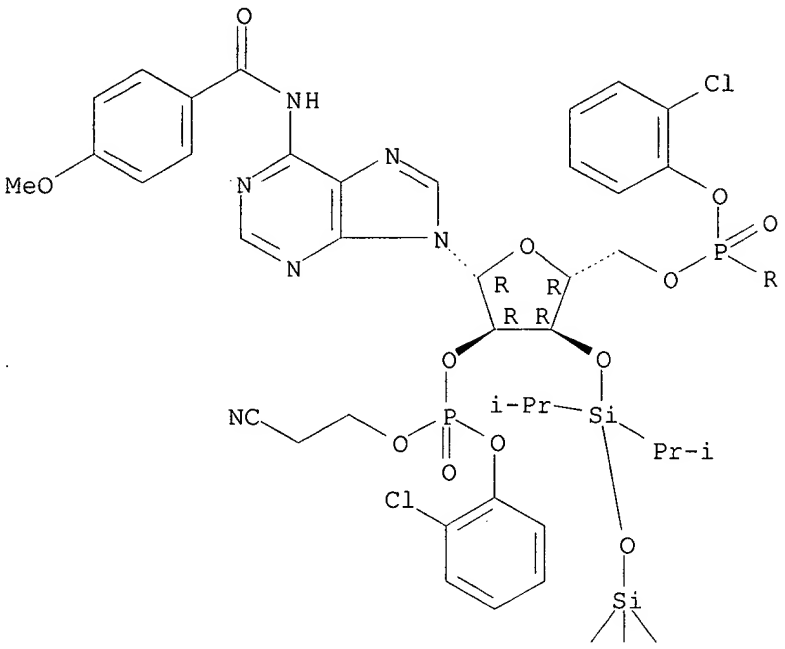


RN 154988-37-1 HCAPLUS
CN 2'-Adenylic acid, P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-3-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-3'-O-[3-hydroxy-1,1,3,3-tetrakis(1-methylethyl)disiloxanyl]-N-(4-

methoxybenzoyl)-, 2-chlorophenyl 2-cyanoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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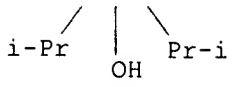
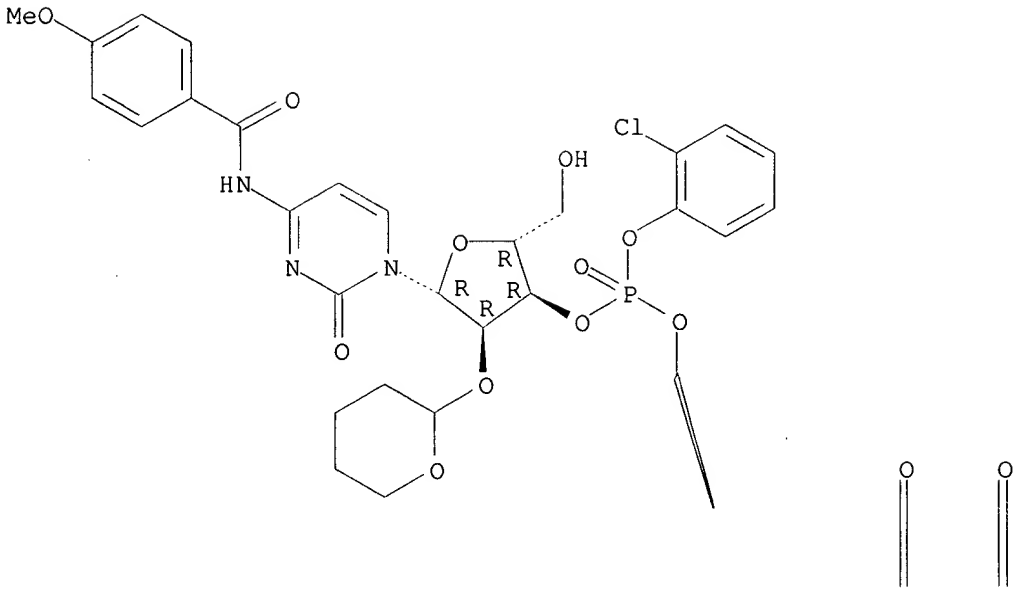
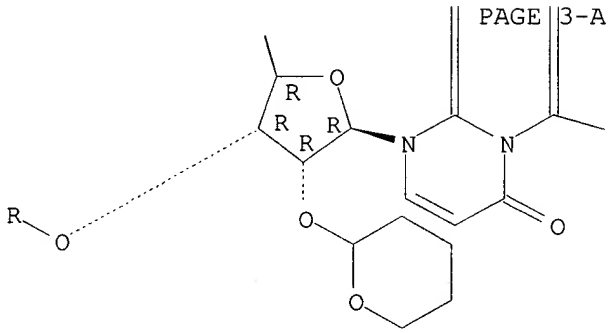



PAGE 3-A

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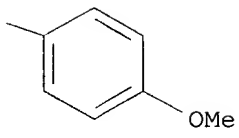


RN 154988-39-3 HCAPLUS

CN 2'-Adenylic acid, P-(2-chlorophenyl)-N-[4-(1,1-dimethylethyl)benzoyl]-6-O-(2-nitrophenyl)-2'-O-(tetrahydro-2H-pyran-2-yl)guanylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-3-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-3'-O-[3-hydroxy-1,1,3,3-tetrakis(1-methylethyl)disiloxanyl]-N-(4-methoxybenzoyl)-, mono(2-chlorophenyl) ester, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

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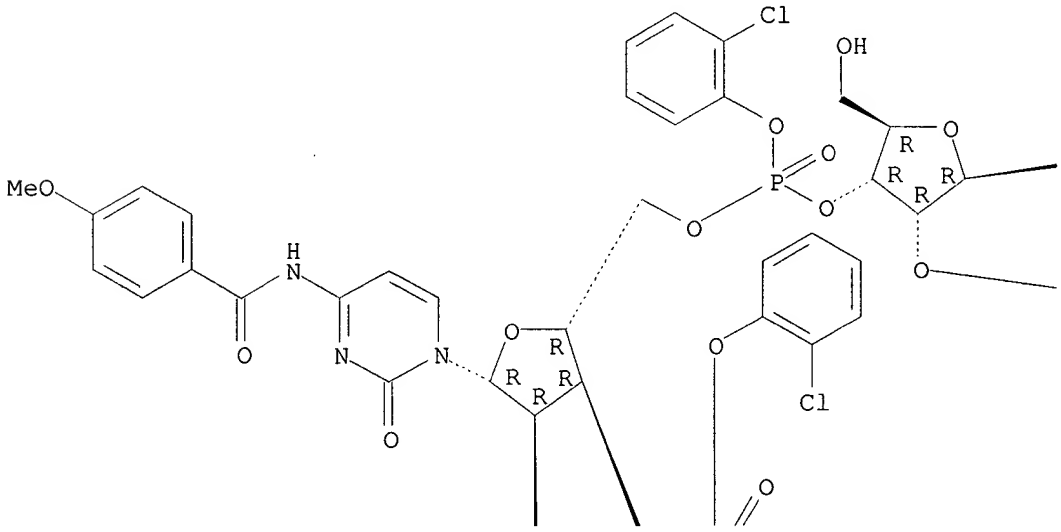
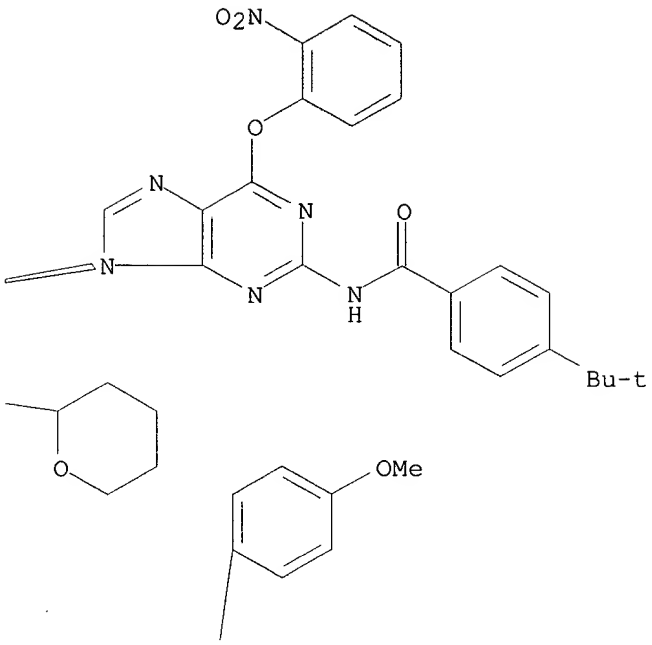
CRN 154988-38-2
CMF C130 H146 Cl4 N16 O43 P4 Si2
CDES 5:ALL,B-D-RIBO

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

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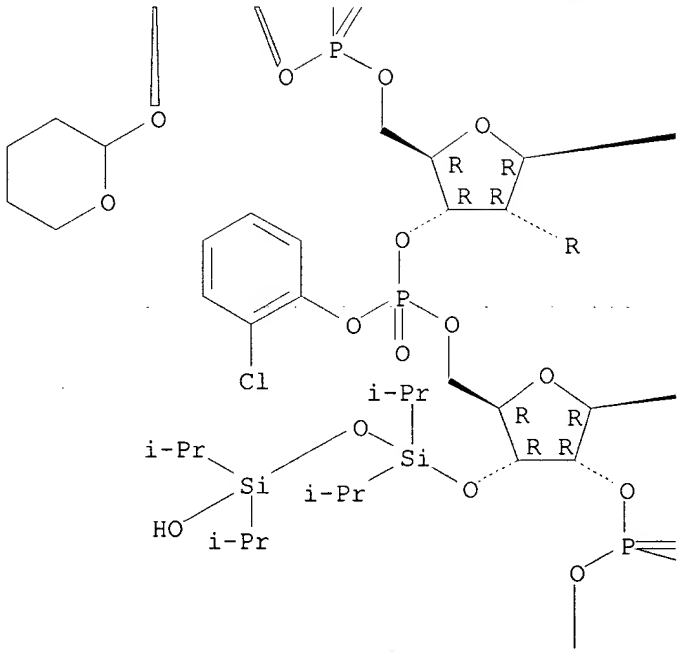

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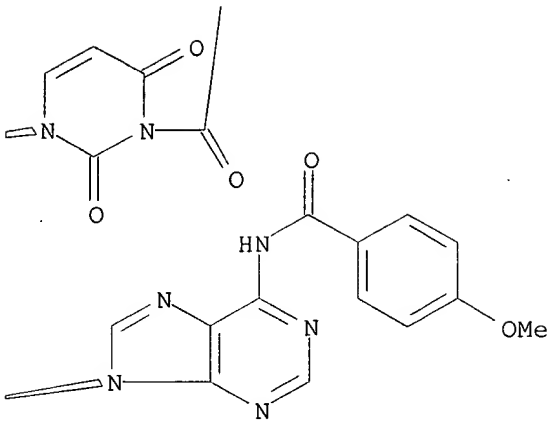

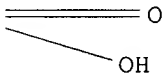

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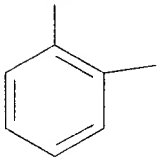

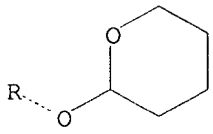

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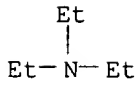
CM 2

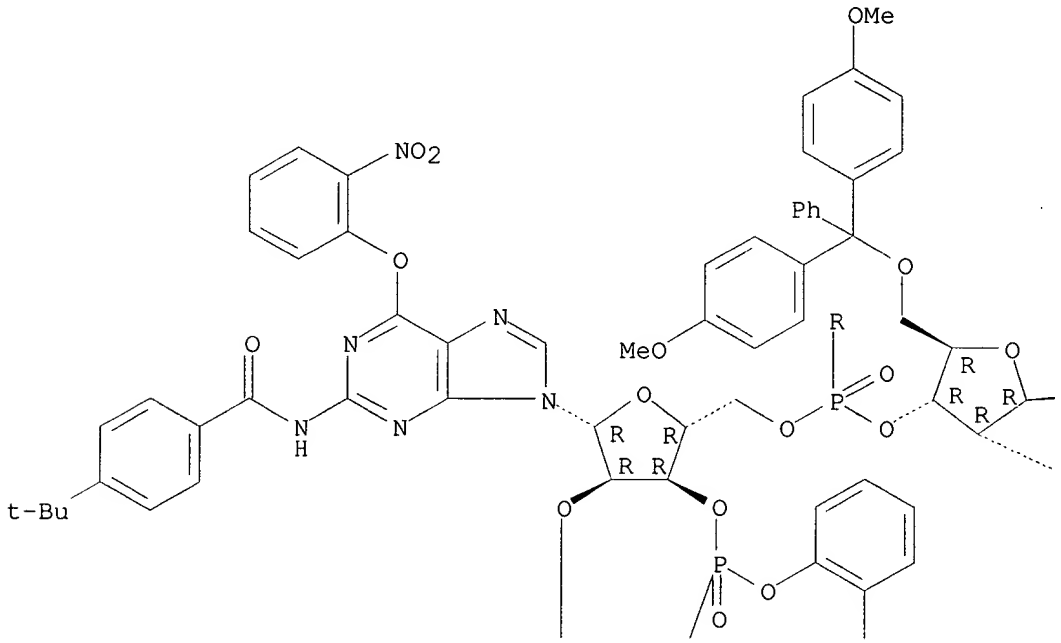
CRN 121-44-8
CMF C6 H15 N



RN 154988-40-6 HCAPLUS
CN 3'-Uridylic acid, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)adenylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-N-[4-(1,1-dimethylethyl)benzoyl]-6-O-(2-nitrophenyl)-2'-O-(tetrahydro-2H-pyran-2-yl)guanylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-3-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)-, 2-chlorophenyl 2-cyanoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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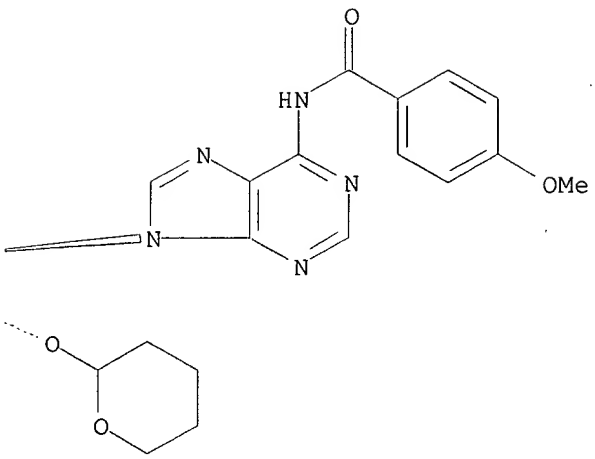

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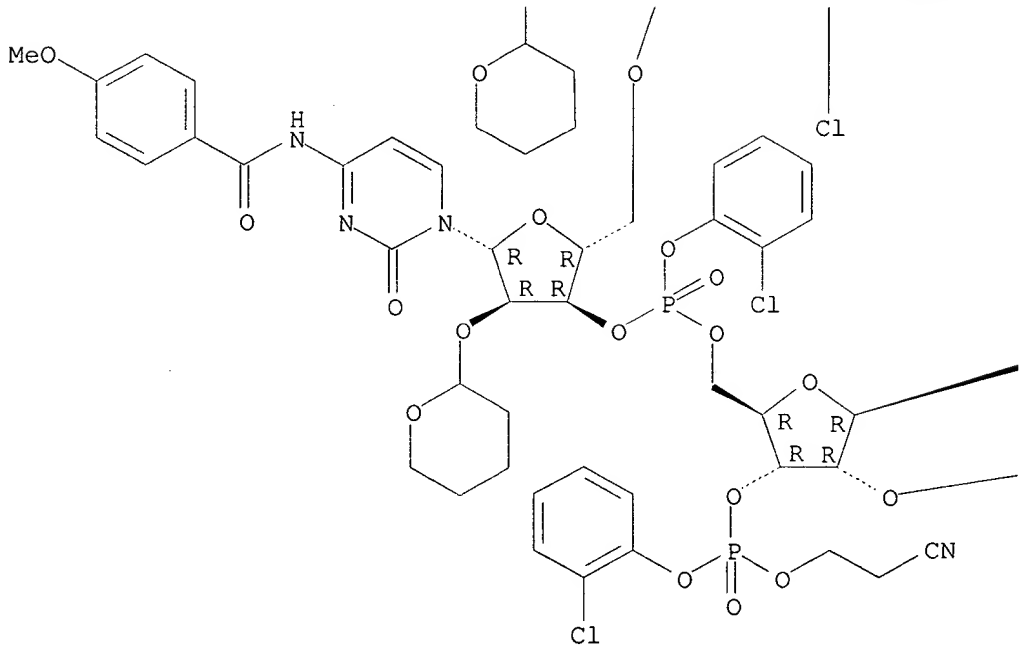
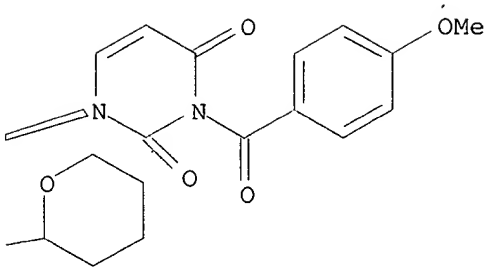


PAGE 2-B

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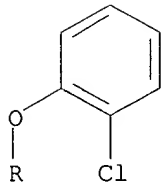


RN 155023-05-5 HCAPLUS
CN 2'-Adenylic acid, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-3-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-3'-O-[3-hydroxy-1,1,3,3-tetrakis(1-methylethyl)disiloxanyl]-N-(4-methoxybenzoyl)-, 2-chlorophenyl 2-cyanoethyl ester (9CI) (CA INDEX NAME)

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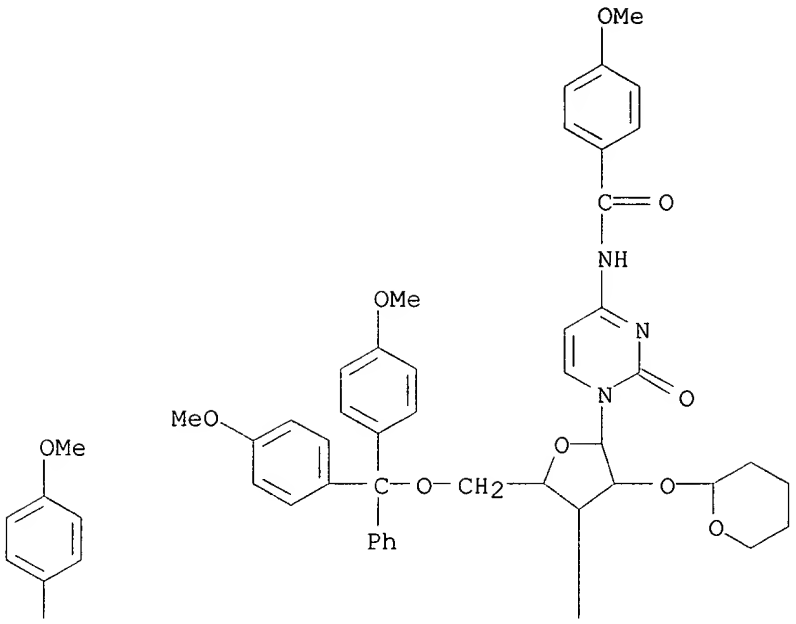

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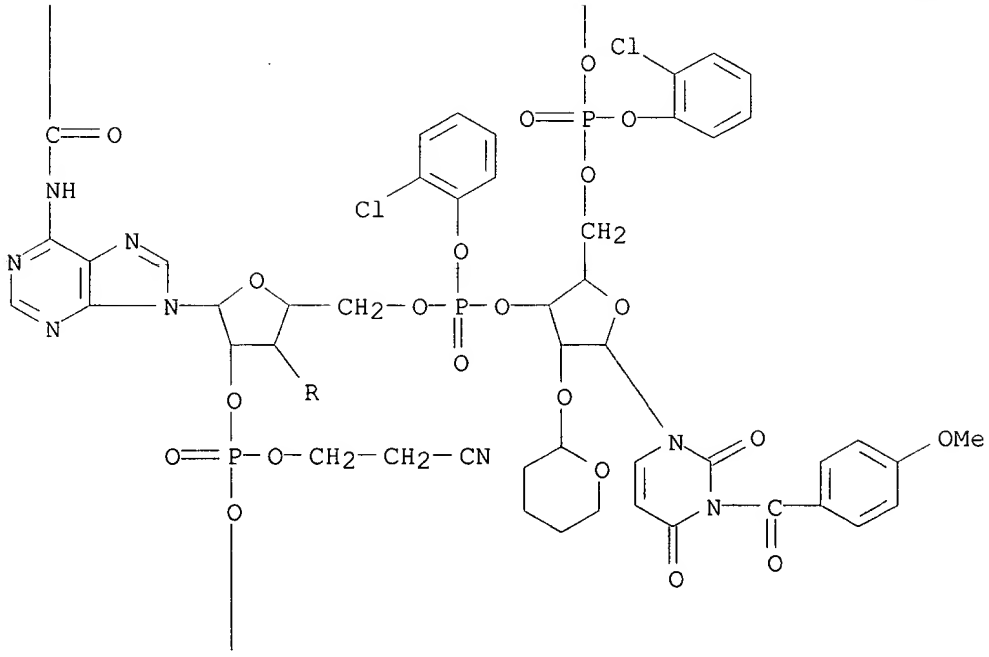

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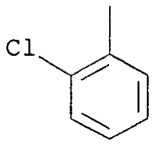
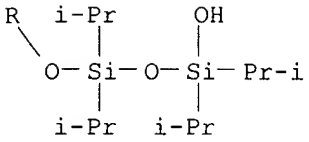
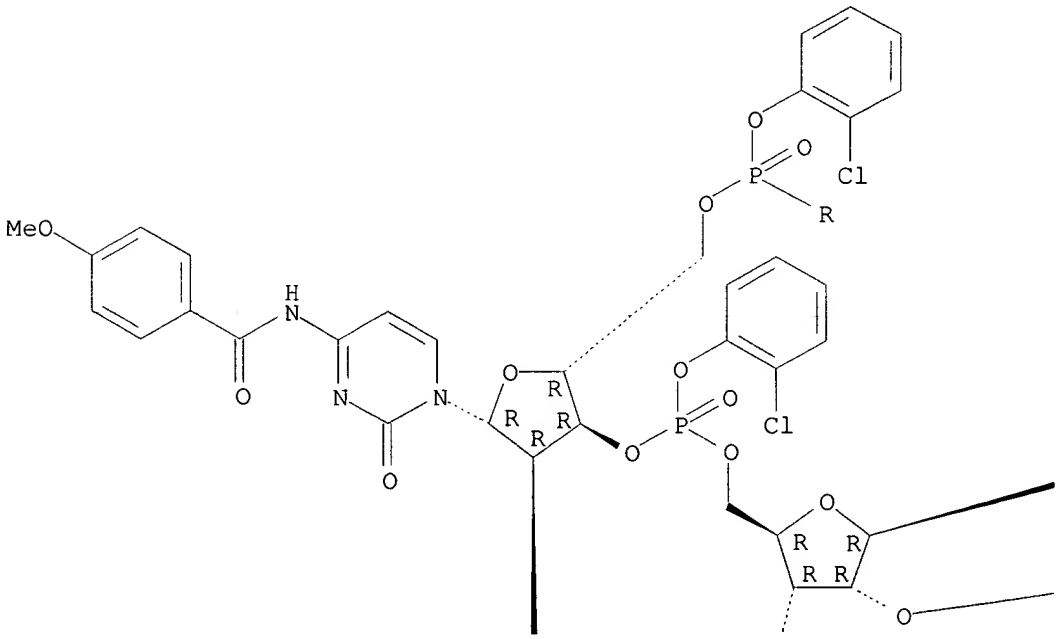



RN 155065-19-3 HCAPLUS
CN 2'-Adenylic acid, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-P-(2-chlorophenyl)-N-[4-(1,1-dimethylethyl)benzoyl]-6-O-(2-nitrophenyl)-2'-O-(tetrahydro-2H-pyran-2-yl)guanylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-3-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-3'-O-[3-hydroxy-1,1,3,3-tetrakis(1-methylethyl)disiloxanyl]-N-(4-methoxybenzoyl)-, 2-chlorophenyl 2-cyanoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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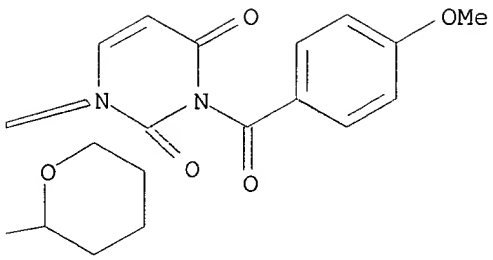


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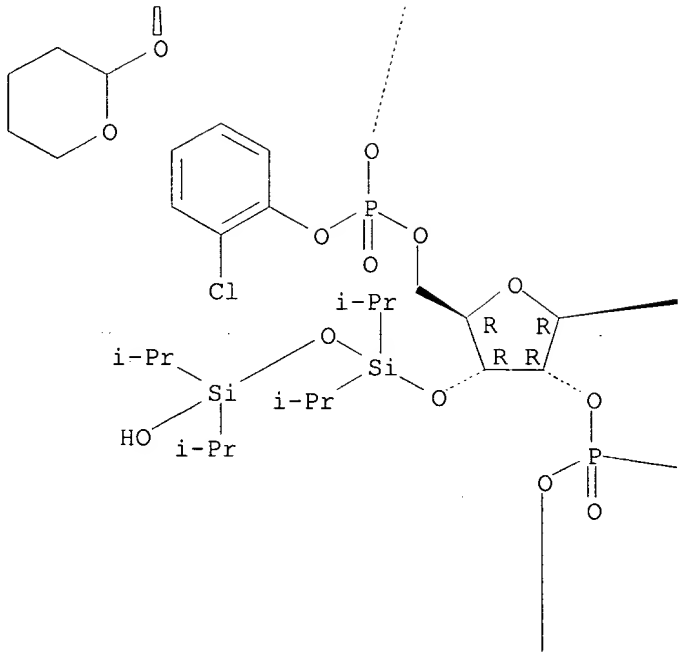

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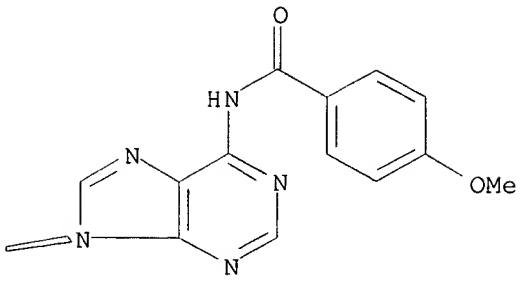

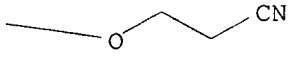

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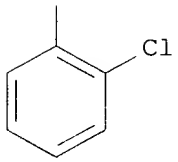

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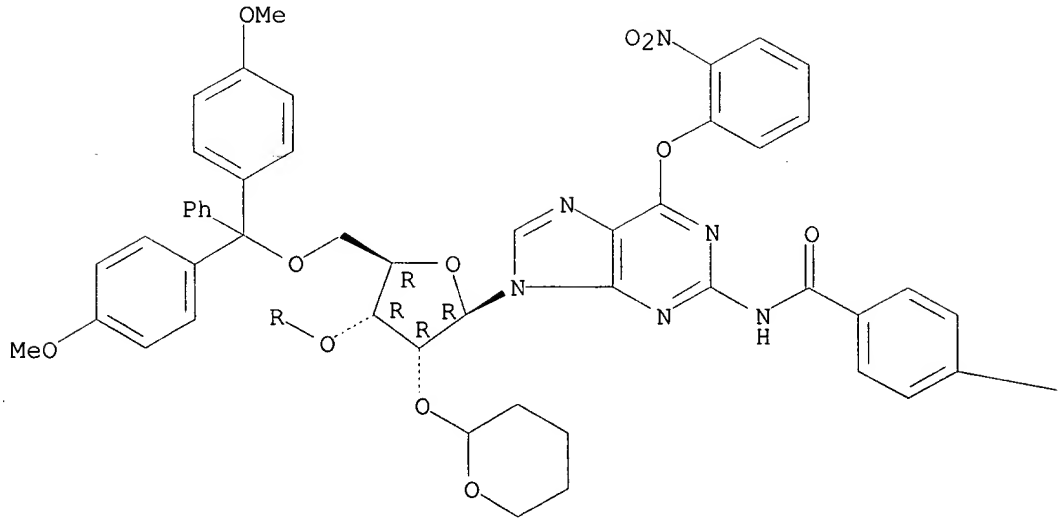
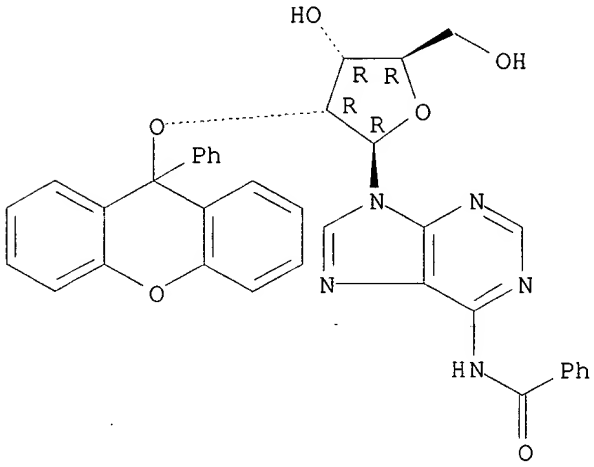


—Bu-t

IT **84315-17-3 147242-12-4 154976-88-2**
**154976-92-8 154988-43-9 154988-44-0**
**154988-46-2**
RL: RCT (Reactant)
(reaction of, in synthesis of oligoribonucleotides lariat RNAs)
RN 84315-17-3 HCAPLUS
CN Adenosine, N-benzoyl-2'-O-(9-phenyl-9H-xanthen-9-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



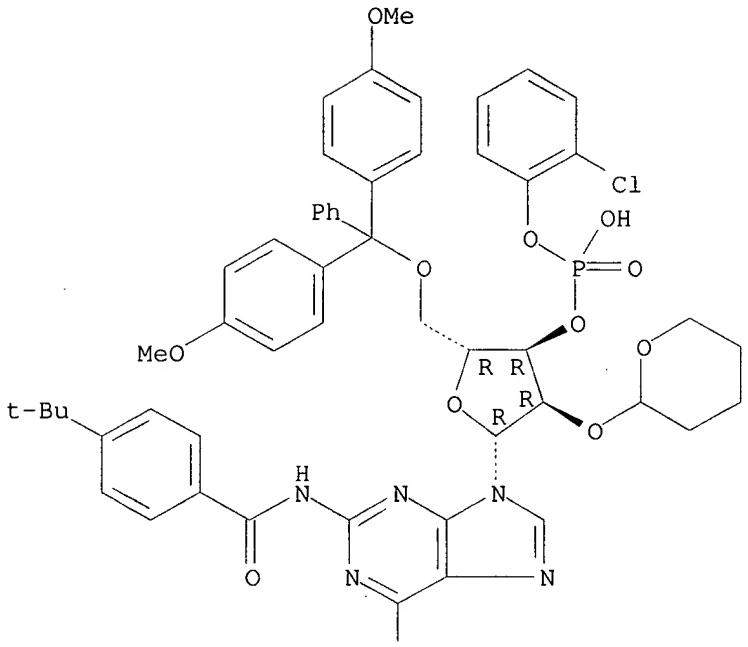

RN 147242-12-4 HCAPLUS
CN 3'-Guanylic acid, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-N-[4-(1,1-dimethylethyl)benzoyl]-6-O-(2-nitrophenyl)-2'-O-(tetrahydro-2H-pyran-2-yl)-, mono(2-chlorophenyl) ester, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

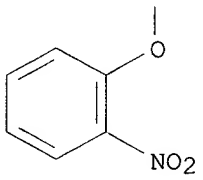
CRN 147242-11-3
CMF C59 H58 Cl N6 O14 P
CDES 5:B-D-RIBO

Absolute stereochemistry.

PAGE 1-A

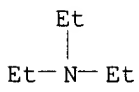



PAGE 2-A




CM 2

CRN 121-44-8
CMF C6 H15 N



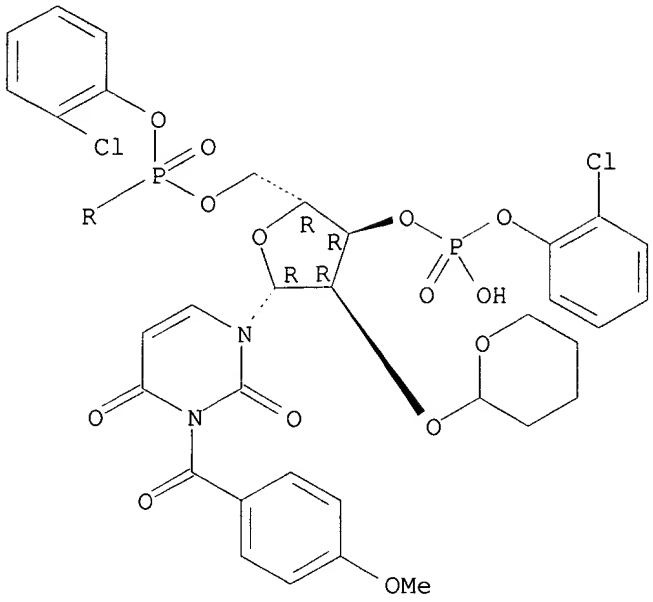

RN 154976-88-2 HCAPLUS
CN 3'-Uridylic acid, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-3-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)-, mono(2-chlorophenyl) ester, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

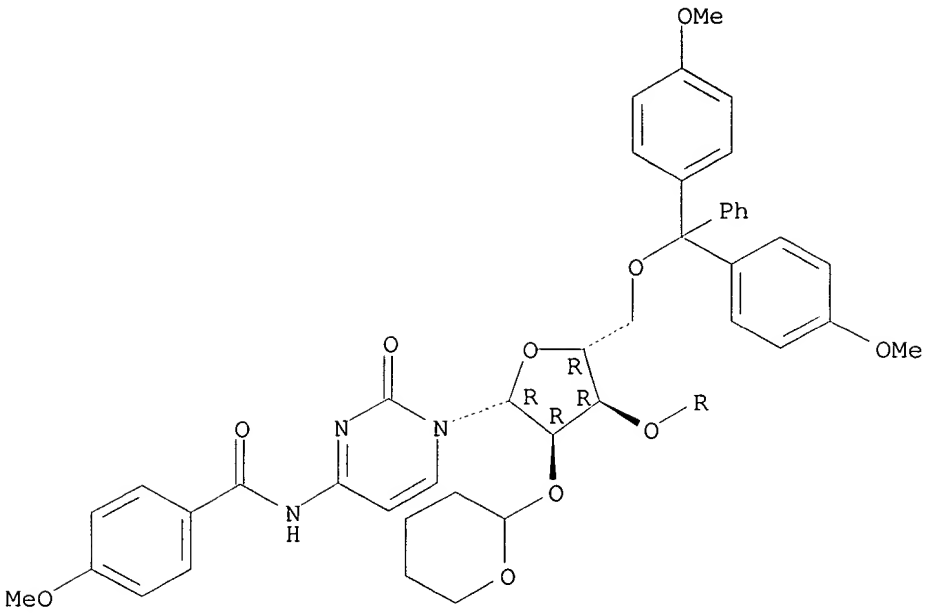
CRN 154976-87-1
CMF C77 H77 Cl2 N5 O24 P2
CDES 5:B-D-RIBO,B-D-RIBO

Absolute stereochemistry.

PAGE 1-A

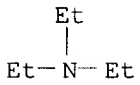


PAGE 2-A




CM 2

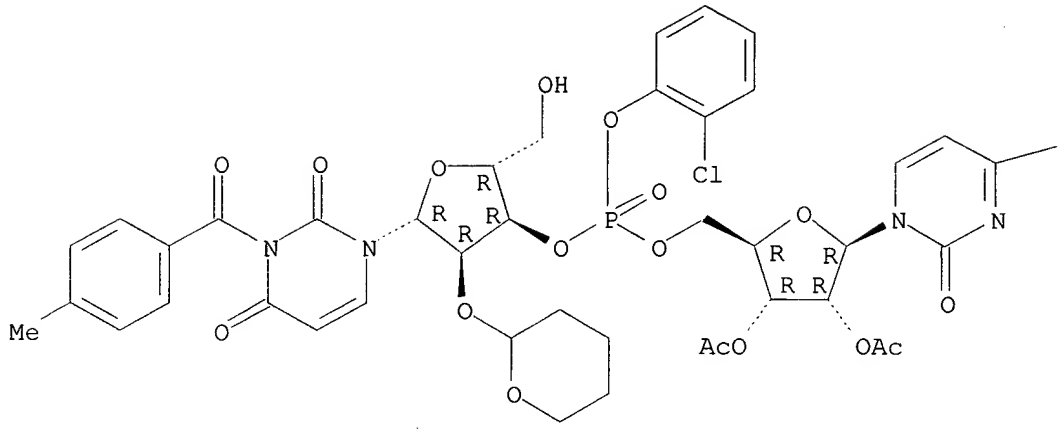
CRN 121-44-8
CMF C6 H15 N



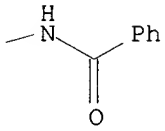

RN 154976-92-8 HCAPLUS
CN Cytidine, P-(2-chlorophenyl)-3-(4-methylbenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-N-benzoyl-, 2',3'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A




PAGE 1-B



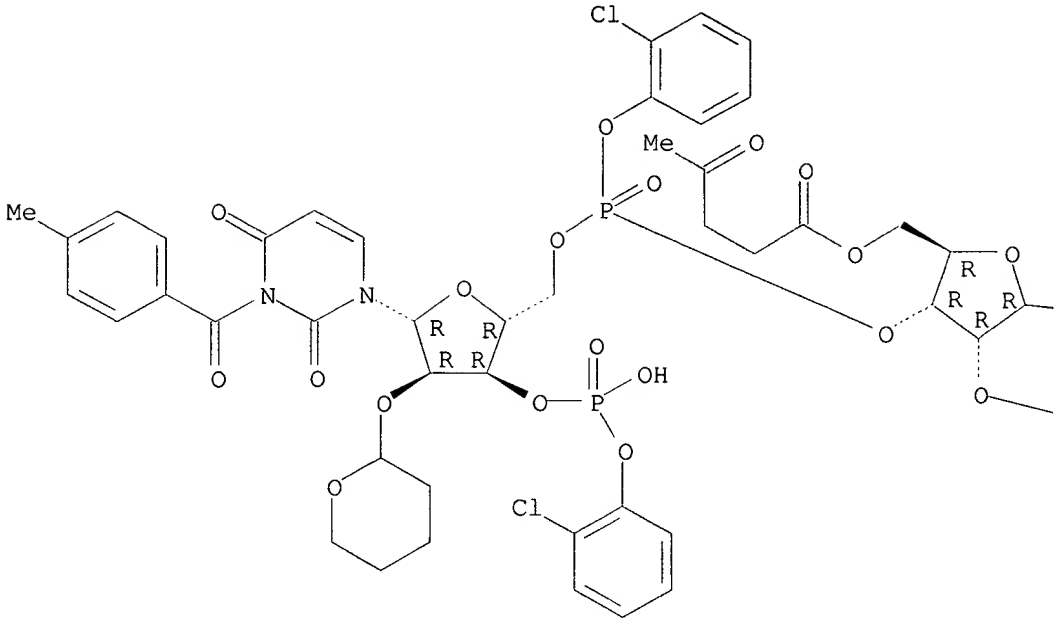

RN 154988-43-9 HCAPLUS
CN 3'-Uridylic acid, N-benzoyl-P-(2-chlorophenyl)-5'-O-(1,4-dioxopentyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-3-(4-methylbenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)-, mono(2-chlorophenyl) ester, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

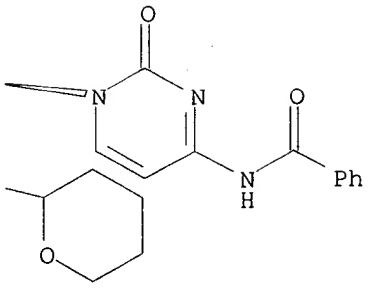
CRN 154988-42-8
CMF C60 H63 Cl2 N5 O22 P2
CDES 5:B-D-RIBO,B-D-RIBO

Absolute stereochemistry.

PAGE 1-A

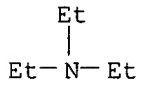


PAGE 1-B



CM 2

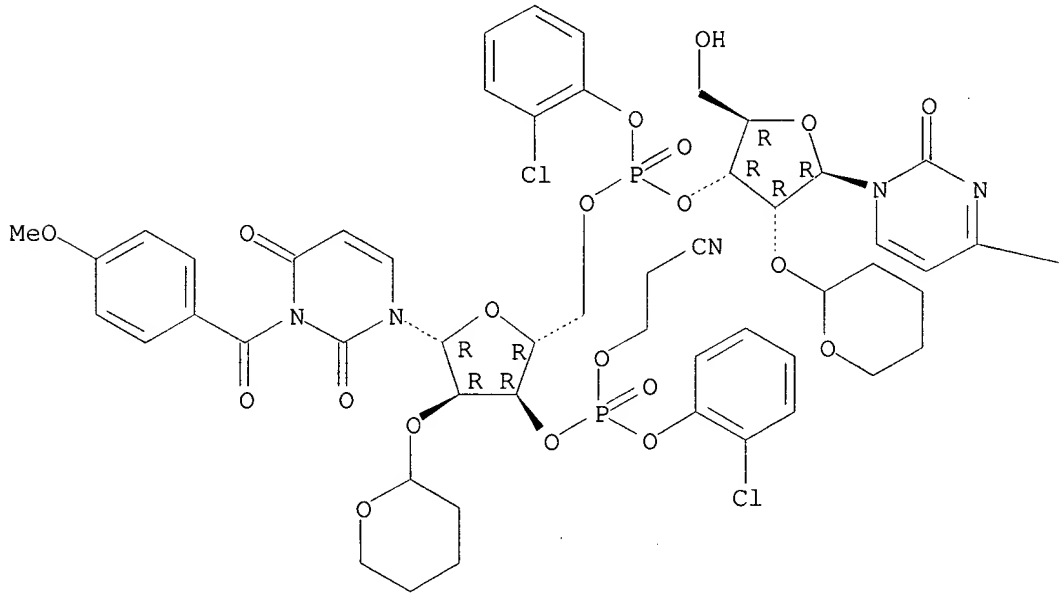
CRN 121-44-8
CMF C6 H15 N



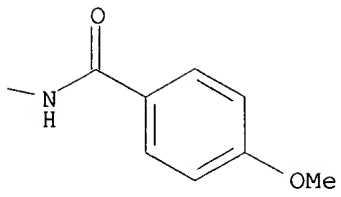
RN 154988-44-0 HCAPLUS
CN 3'-Uridylic acid, P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-3-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)-, 2-chlorophenyl 2-cyanoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



RN 154988-46-2 HCAPLUS

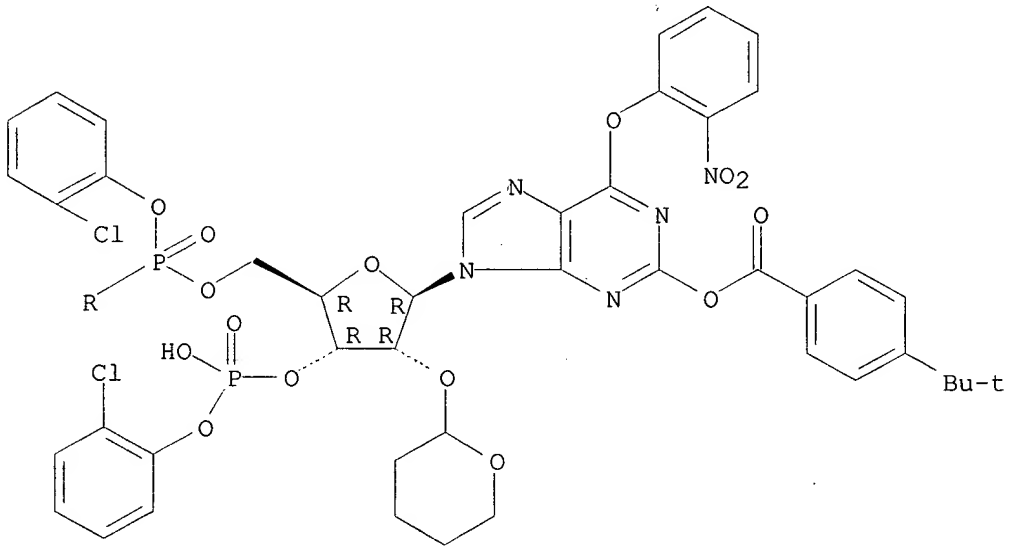
CN 3'-Xanthylic acid, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-P-(2-chlorophenyl)-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)adenylyl-(3'.fwdarw.5')-6-O-(2-nitrophenyl)-2'-O-(tetrahydro-2H-pyran-2-yl)-, mono(2-chlorophenyl) ester, 2-[4-(1,1-dimethylethyl)benzoate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

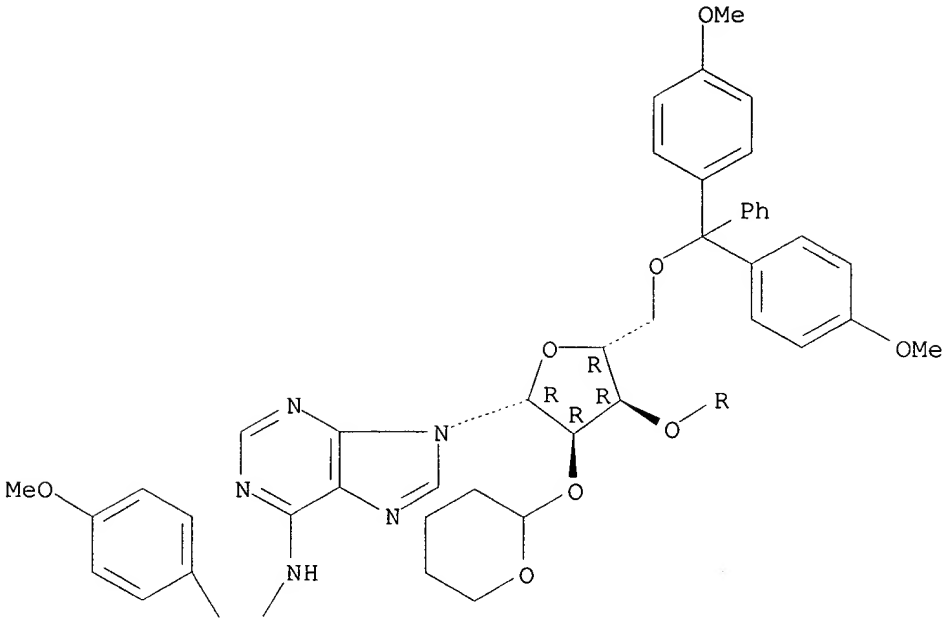
CRN 154988-45-1
CMF C88 H86 Cl2 N10 O24 P2
CDES 5:B-D-RIBO,B-D-RIBO

Absolute stereochemistry.

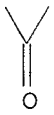
PAGE 1-A



PAGE 2-A

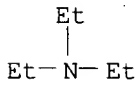



PAGE 3-A




CM 2

CRN 121-44-8
CMF C6 H15 N

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L39 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
CC 33-9 (Carbohydrates)
ST oligoribonucleotide lariat RNA self bond cleavage; nucleotide oligoribo lariat RNA bond cleavage; conformation thermodn cyclic oligoribonucleotide lariat RNA; mol dynamics simulation cyclic oligoribonucleotide prepn
IT Conformation and Conformers

(of cyclic oligoribonucleotides lariat-RNAs)
IT Simulation and Modeling, physicochemical
(mol. dynamics, of cyclic oligoribonucleotides lariat-RNAs)
IT Nucleotides, preparation
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(oligo-, cyclic, lariat-RNAs, prepn., conformation, and self-cleavage of)
IT 147242-27-1
RL: PRP (Properties); RCT (Reactant)
(conformation and self-cleavage of)
IT 154976-71-3P 154976-72-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conformation of)
IT **154976-73-5P** 154976-74-6P **154976-75-7P**
**154976-77-9P 154976-78-0P 154976-80-4P**
**154976-82-6P 154976-84-8P 154976-85-9P**
**154976-86-0P** 154976-89-3P **154988-37-1P**
**154988-39-3P 154988-40-6P** 154988-41-7P 154999-04-9P
154999-05-0P 154999-06-1P **155023-05-5P 155065-19-3P**
155833-31-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in synthesis of oligoribonucleotides lariat RNAs)
IT 150829-18-8P 154976-69-9P 154976-70-2P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., conformation, and self-cleavage of)
IT 1129-37-9 72351-28-1 74257-00-4 **84315-17-3** 102690-88-0
**147242-12-4 154976-88-2** 154976-91-7
**154976-92-8** 154976-93-9 **154988-43-9**
**154988-44-0 154988-46-2**
RL: RCT (Reactant)
(reaction of, in synthesis of oligoribonucleotides lariat RNAs)

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L39 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
AB . . . exists as two conformers (A and B) in slow exchange on the NMR time scale. The loop nucleotides in the **B-form** of the hexamer have ribose, glycoside bonds and phosphate backbone conformation. Torsonal constraints derived form 1H-1H, 1H-31P and 13C-31P coupling. . .
IT **154976-73-5P** 154976-74-6P **154976-75-7P**
**154976-77-9P 154976-78-0P 154976-80-4P**
**154976-82-6P 154976-84-8P 154976-85-9P**
**154976-86-0P** 154976-89-3P **154988-37-1P**
**154988-39-3P 154988-40-6P** 154988-41-7P 154999-04-9P
154999-05-0P 154999-06-1P **155023-05-5P 155065-19-3P**
155833-31-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in synthesis of oligoribonucleotides lariat RNAs)
IT 1129-37-9 72351-28-1 74257-00-4 **84315-17-3** 102690-88-0
**147242-12-4 154976-88-2** 154976-91-7
**154976-92-8** 154976-93-9 **154988-43-9**
**154988-44-0 154988-46-2**
RL: RCT (Reactant)
(reaction of, in synthesis of oligoribonucleotides lariat RNAs)

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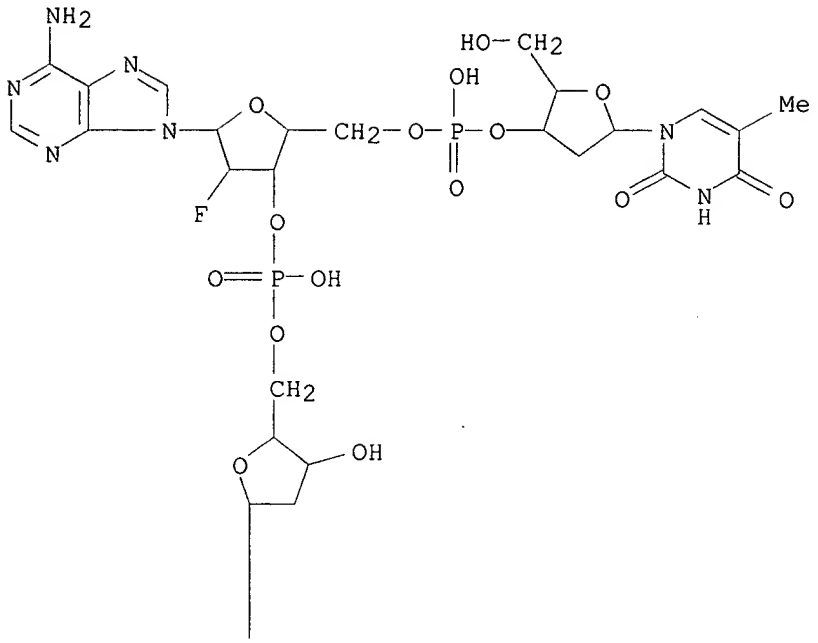
L39 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1993:517734 HCAPLUS
DOCUMENT NUMBER: 119:117734
TITLE: Uniformly modified 2'-deoxy-2'-fluoro-phosphorothioate oligonucleotides as nuclease-resistant antisense compounds with high affinity and specificity for RNA targets
AUTHOR(S): Kawasaki, Andrew M.; Casper, Martin D.; Freier, Susan M.; Lesnik, Elena A.; Zounes, Maryann C.; Cummins, Lendell L.; Gonzalez, Carolyn; Cook, P. Dan
CORPORATE SOURCE: ISIS Pharm., Carlsbad, CA, 92008, USA
SOURCE: J. Med. Chem. (1993), 36(7), 831-41
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

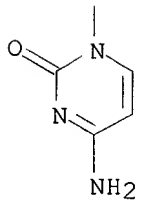
AB "Uniformly" modified phosphodiester or phosphorothioate oligonucleotides incorporating 2'- deoxy-2'-fluoroadenosine, -guanosine, -uridine, and -cytidine, reported herein for the first time, when hybridized with RNA afforded consistent additive enhancement of duplex stability without compromising base-pair specificity. CD spectra of the 2'-deoxy-2'-fluoro-modified oligonucleotides hybridized with RNA indicated that the duplex adopts a fully **A-form** conformation.
The 2'-deoxy-2'-fluoro-modified oligonucleotides in phosphodiester form were not resistant to nucleases; however, the modified phosphorothioate oligonucleotides were highly nuclease resistant and retained exceptional binding affinity to the RNA targets. The stabilizing effects of the 2'-deoxy-2'-fluoro modifications on RNA-DNA duplexes were shown to be superior to those of the 2'-O-methylribo substitutions. "Uniformly" modified 2'-deoxy-2'-fluoro phosphorothioate oligonucleotides afforded antisense mols. with high binding affinity for the RNA target and stability toward nucleases.

IT **146954-70-3P 146954-71-4P 146954-72-5P**
**146954-73-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and NMR spectra of, proton)
RN 146954-70-3 HCAPLUS
CN Cytidine, thymidylyl-(3'.fwdarw.5')-2'-deoxy-2'-fluoroadenylyl-(3'.fwdarw.5')-2'-deoxy- (9CI) (CA INDEX NAME)

PAGE 1-A

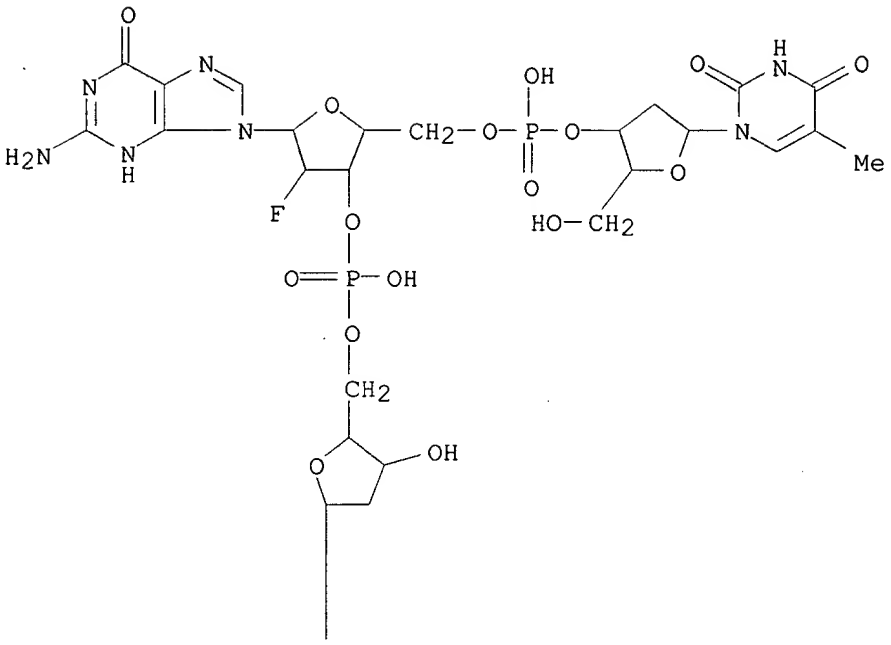


PAGE 2-A

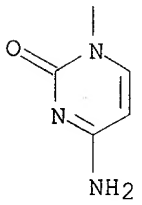


RN 146954-71-4 HCAPLUS
CN Cytidine, thymidylyl-(3'.fwdarw.5')-2'-deoxy-2'-fluoroguanylyl-(3'.fwdarw.5')-2'-deoxy- (9CI) (CA INDEX NAME)

PAGE 1-A

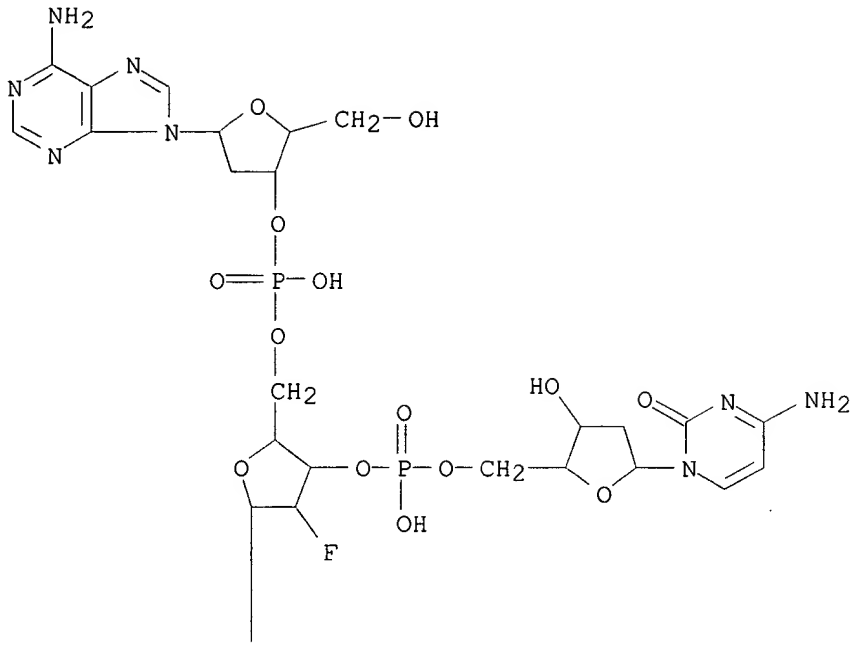


PAGE 2-A

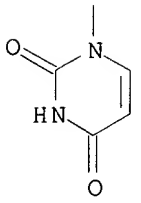


RN 146954-72-5 HCAPLUS
CN Cytidine, 2'-deoxyadenylyl-(3'.fwdarw.5')-2'-deoxy-2'-fluorouridylyl-(3'.fwdarw.5')-2'-deoxy- (9CI) (CA INDEX NAME)

PAGE 1-A

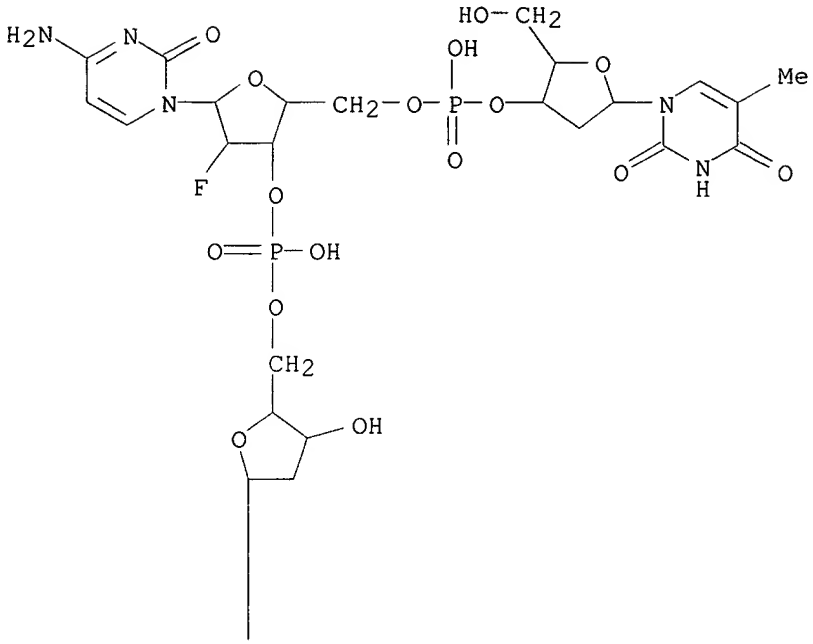


PAGE 2-A

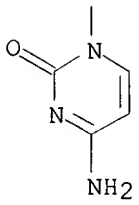


RN 146954-73-6 HCAPLUS
CN Cytidine, thymidylyl-(3'.fwdarw.5')-2'-deoxy-2'-fluorocytidylyl-(3'.fwdarw.5')-2'-deoxy- (9CI) (CA INDEX NAME)

PAGE 1-A

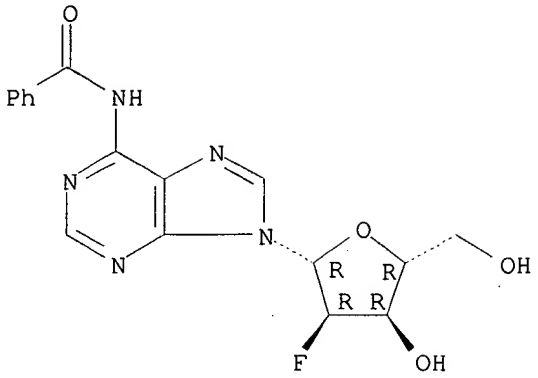


PAGE 2-A



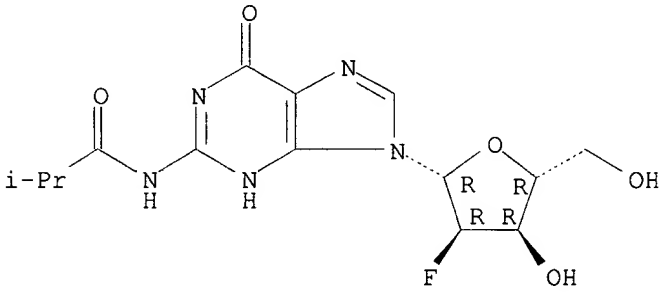
IT **136834-20-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzoylation of)
RN 136834-20-3 HCAPLUS
CN Adenosine, N-benzoyl-2'-deoxy-2'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



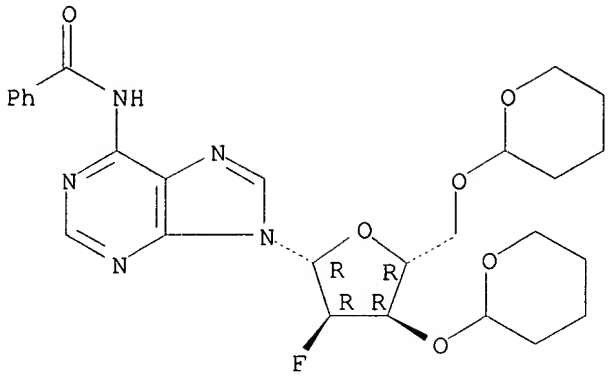
IT **80681-25-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deblocking of)
RN 80681-25-0 HCAPLUS
CN Guanosine, 2'-deoxy-2'-fluoro-N-(2-methyl-1-oxopropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



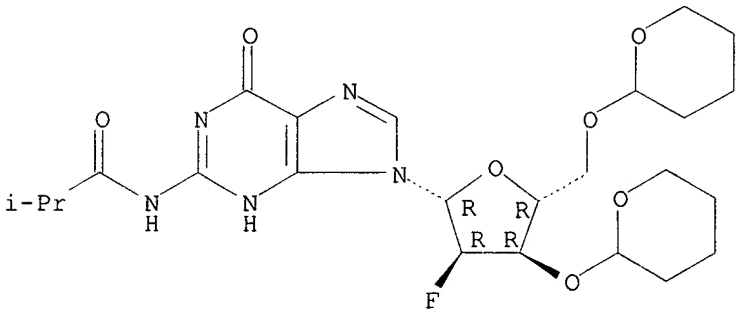
IT **146954-64-5P 146954-69-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and partial deblocking of)
RN 146954-64-5 HCAPLUS
CN Adenosine, N-benzoyl-2'-deoxy-2'-fluoro-3',5'-bis-O-(tetrahydro-2H-pyran-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



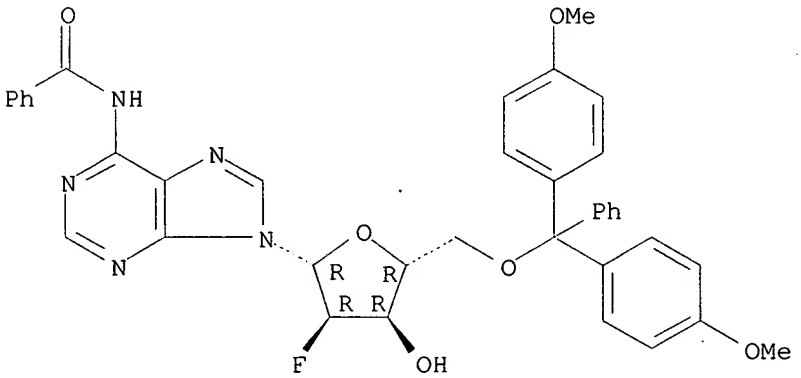
RN 146954-69-0 HCAPLUS
CN Guanosine, 2'-deoxy-2'-fluoro-N-(2-methyl-1-oxopropyl)-3',5'-bis-O-(tetrahydro-2H-pyran-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



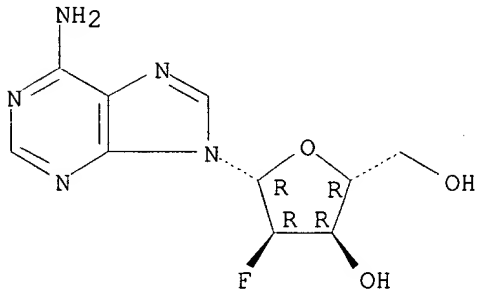
IT **136834-21-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and phosphoramidation of)
RN 136834-21-4 HCAPLUS
CN Adenosine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-2'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



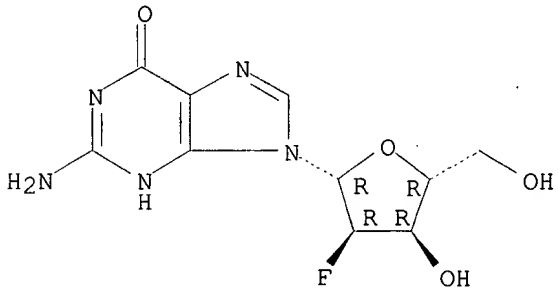
IT **64183-27-3P 78842-13-4P 136834-22-5P**
**144089-96-3P 144089-97-4P 146954-74-7P**
**146954-75-8P 146954-76-9P 146954-77-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in synthesis of DNA)
RN 64183-27-3 HCAPLUS
CN Adenosine, 2'-deoxy-2'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



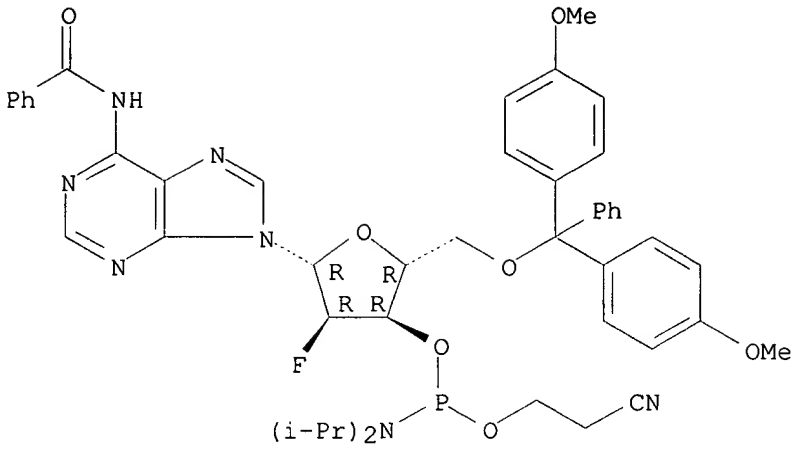
RN 78842-13-4 HCAPLUS
CN Guanosine, 2'-deoxy-2'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



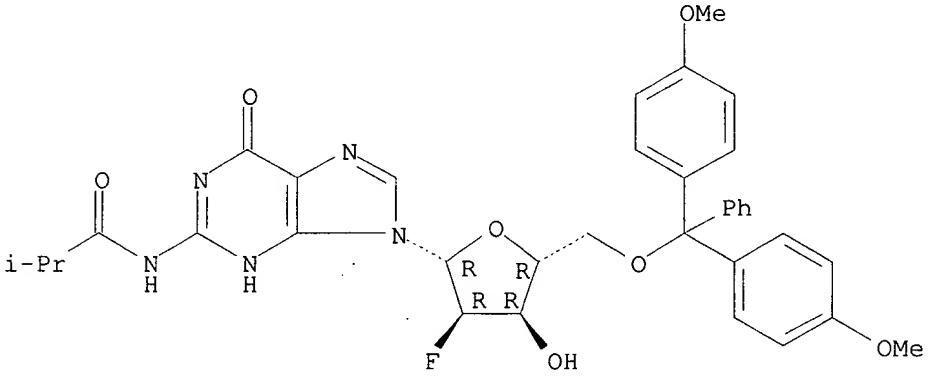
RN 136834-22-5 HCAPLUS
CN Adenosine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-2'-fluoro-, 3'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



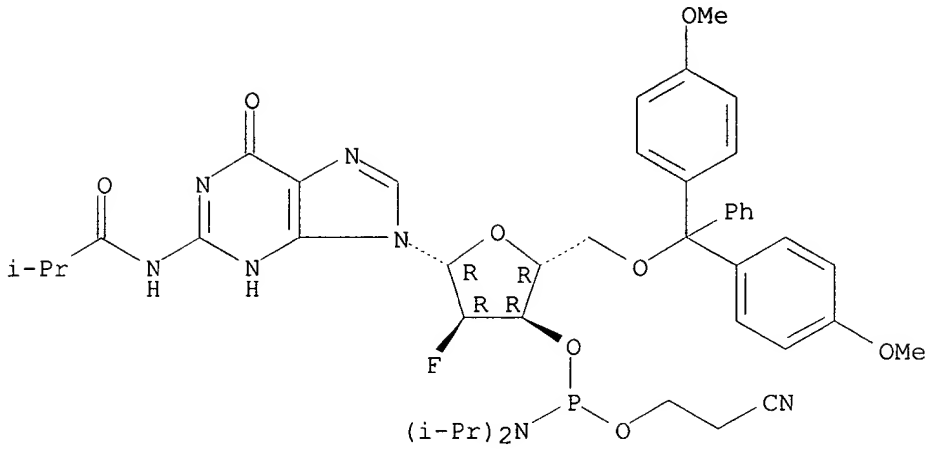
RN 144089-96-3 HCAPLUS
CN Guanosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-2'-fluoro-N-(2-methyl-1-oxopropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



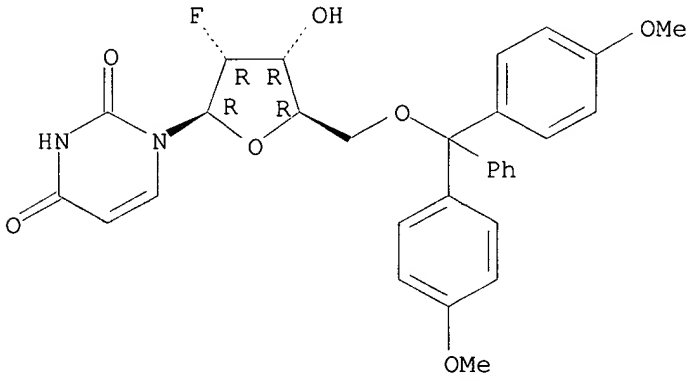
RN 144089-97-4 HCAPLUS
CN Guanosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-2'-fluoro-N-(2-methyl-1-oxopropyl)-, 3'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



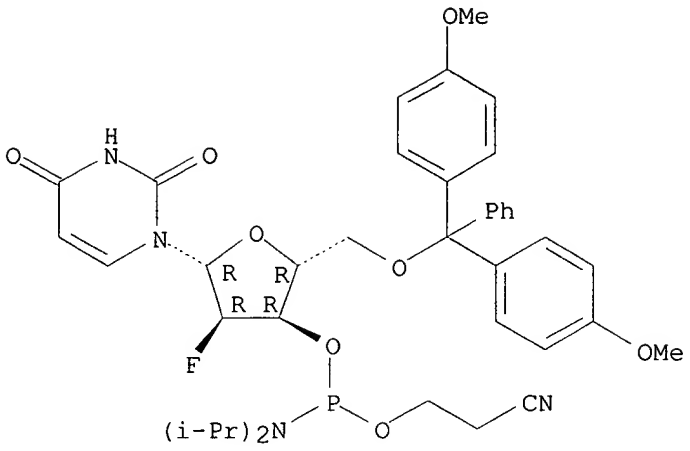
RN 146954-74-7 HCAPLUS
CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-2'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



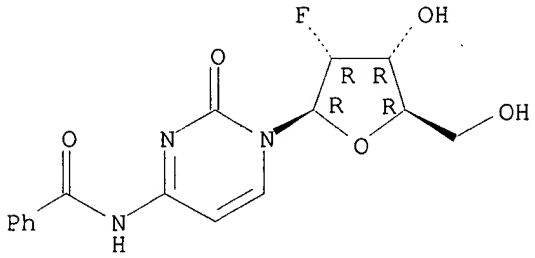
RN 146954-75-8 HCAPLUS
CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-2'-fluoro-, 3'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



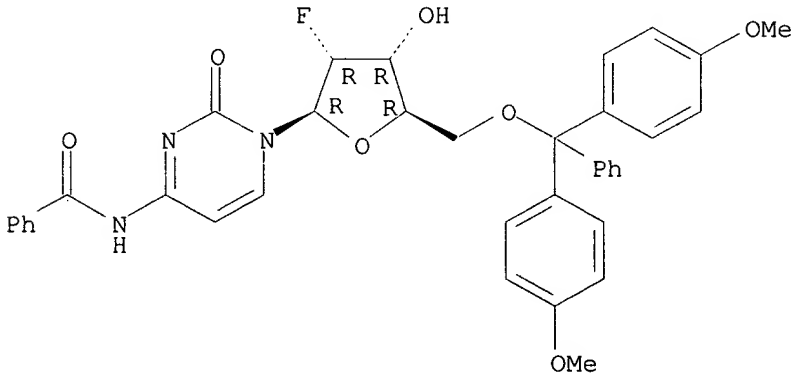
RN 146954-76-9 HCAPLUS
CN Cytidine, N-benzoyl-2'-deoxy-2'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 146954-77-0 HCAPLUS
CN Cytidine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-2'-fluoro- (9CI) (CA INDEX NAME)

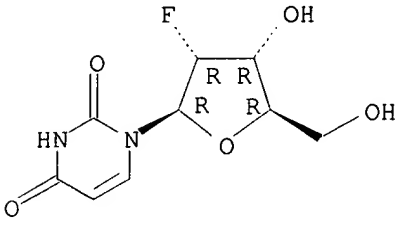
Absolute stereochemistry.



IT **784-71-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and tritylation of)

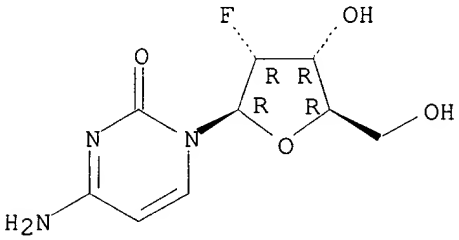
RN 784-71-4 HCAPLUS
CN Uridine, 2'-deoxy-2'-fluoro- (7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **10212-20-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and N-benzoylation of)
RN 10212-20-1 HCAPLUS
CN Cytidine, 2'-deoxy-2'-fluoro- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d ind

L39 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
CC 33-9 (Carbohydrates)
ST oligoribonucleotide lariat RNA self bond cleavage; nucleotide oligoribo lariat RNA bond cleavage; conformation thermodn cyclic oligoribonucleotide lariat RNA; mol dynamics simulation cyclic oligoribonucleotide prepn
IT Conformation and Conformers
(of cyclic oligoribonucleotides lariat-RNAs)
IT Simulation and Modeling, physicochemical
(mol. dynamics, of cyclic oligoribonucleotides lariat-RNAs)
IT Nucleotides, preparation
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(oligo-, cyclic, lariat-RNAs, prepn., conformation, and self-cleavage of)
IT 147242-27-1
RL: PRP (Properties); RCT (Reactant)
(conformation and self-cleavage of)
IT 154976-71-3P 154976-72-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conformation of)
IT **154976-73-5P** 154976-74-6P **154976-75-7P**
**154976-77-9P 154976-78-0P 154976-80-4P**

=> d ind 2

indexing

L39 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS
CC 33-10 (Carbohydrates)
Section cross-reference(s): 6, 7, 9, 22
ST deoxyfluorophosphorothioate oligonucleotide nuclease resistant antisense; RNA DNA duplex deoxyfluorophosphorothioate; phosphorothioate oligonucleotide nuclease resistant antisense; nucleotide oligo phosphorothioate nuclease resistant antisense; hybridization thermodn RNA DNA duplex
IT Deoxyribonucleic acids
Ribonucleic acids
RL: SPN (Synthetic preparation); PREP (Preparation)
(2'-deoxy-2'-fluoro, phosphorothioate-contg., prepn. and effects of, on DNA-RNA duplex stability)
IT Ribonucleic acids
RL: RCT (Reactant)
(duplex of, with DNA, effect of antisense sequences on stability of)
IT Deoxyribonucleic acids
RL: RCT (Reactant)
(duplex of, with RNA, effect of antisense sequences on stability of)
IT 136796-53-7 149149-13-3 149149-14-4 149593-79-3 149593-80-6
149593-81-7 149593-82-8 149593-83-9 149593-84-0 149593-85-1
149593-86-2 149593-87-3 149593-88-4 149593-89-5 149593-90-8
149593-91-9 149593-92-0 149593-93-1 149593-94-2 149593-95-3
149593-97-5 149593-98-6 149593-99-7 149594-00-3 149594-01-4
149594-02-5 149594-03-6 149594-04-7 149594-05-8 149594-06-9
149594-07-0 149594-08-1
RL: PRP (Properties)
(effects of, on DNA-RNA duplex stability)
IT 9026-81-7, Nuclease
RL: RCT (Reactant)
(hydrolysis of DNA and RNA in presence of)
IT 79896-97-2
RL: PROC (Process)
(partial protection of)
IT **146954-70-3P 146954-71-4P 146954-72-5P**
**146954-73-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and NMR spectra of, proton)
IT **136834-20-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzoylation of)
IT **80681-25-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deblocking of)
IT 146954-65-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and desilylation of)
IT 149594-09-2P 149594-10-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and enzymic hydrolysis of)
IT **146954-64-5P** 146954-67-8P **146954-69-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and partial deblocking of)
IT **136834-21-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and phosphoramidation of)
IT **64183-27-3P 78842-13-4P 136834-22-5P**

**144089-96-3P 144089-97-4P** 146954-66-7P
**146954-74-7P 146954-75-8P 146954-76-9P**
**146954-77-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in synthesis of DNA)

IT 136834-18-9P 146954-68-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sequential triflation and fluorination of)

IT **784-71-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and tritylation of)

IT **10212-20-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and N-benzoylation of)

IT 129835-17-2
RL: RCT (Reactant)
(reaction of, in synthesis of DNA)

IT 69304-44-5
RL: RCT (Reactant)
(reaction of, in synthesis of DNA and RNA)

IT 69304-44-5
RL: RCT (Reactant)
(reaction of, in synthesis of DNA and RNA)

=> d kwic 2

L39 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS
AB . . . without compromising base-pair specificity. CD spectra of the 2'-deoxy-2'-fluoro-modified oligonucleotides hybridized with RNA indicated that the duplex adopts a fully **A-form** conformation. The 2'-deoxy-2'-fluoro-modified oligonucleotides in phosphodiester form were not resistant to nucleases; however, the modified phosphorothioate oligonucleotides were highly nuclease. . .

IT **146954-70-3P 146954-71-4P 146954-72-5P**
**146954-73-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and NMR spectra of, proton)

IT **136834-20-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzoylation of)

IT **80681-25-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deblocking of)

IT **146954-64-5P** 146954-67-8P **146954-69-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and partial deblocking of)

IT **136834-21-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and phosphoramidation of)

IT **64183-27-3P 78842-13-4P 136834-22-5P**
**144089-96-3P 144089-97-4P** 146954-66-7P
**146954-74-7P 146954-75-8P 146954-76-9P**
**146954-77-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in synthesis of DNA)

IT **784-71-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and tritylation of)

IT **10212-20-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and N-benzoylation of)

STR search

KRISHNAN 09/970,971

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L12             1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  2000:790526/AN
L13               STR
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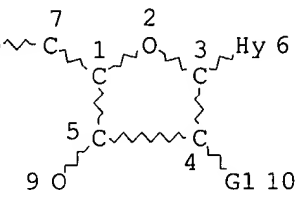
same STR as for L39

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                                 @11 12        @13 14  15  16      @17 @18

 Ak O N          O G3 Ak O
@20 21 @22       @23 24  25  26

VAR G1=13/23/11/F
REP G2=(1-10) 17-13 18-15
REP G3=(1-10) 20-23 22-25
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT   6
GGCAT   IS LIN  SAT  AT  15
GGCAT   IS LIN  SAT  AT  17
GGCAT   IS LIN  SAT  AT  20
GGCAT   IS LIN  SAT  AT  25
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M4 C  AT   6
ECOUNT  IS X10 C  AT  15
ECOUNT  IS M2-X10 C  AT  17
ECOUNT  IS M2-X10 C  AT  20
ECOUNT  IS X10 C  AT  25

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  25

STEREO ATTRIBUTES: NONE
L16          5085 SEA FILE=REGISTRY SSS FUL L13
L17           858 SEA FILE=REGISTRY ABB=ON  PLU=ON  L16 AND NCNC3/ES AND
                  NCNC2-NCNC3/ES
L18           858 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 AND P/ELS
L19          4227 SEA FILE=REGISTRY ABB=ON  PLU=ON  L16 NOT L18
L20           222 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L18
L21          2311 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19
L30         19435 SEA FILE=HCAPLUS ABB=ON  PLU=ON  A"-"FORM
L31          2857 SEA FILE=HCAPLUS ABB=ON  PLU=ON  B"-"FORM
L32             3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 AND L20
L33             7 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 AND L21
L34             4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L31 AND L20
L35             5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L31 AND L21
L38             2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L32 OR L34) AND (L33 OR L35)

L39             2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L38 NOT L12
L40        182405 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "A AND B"
L41            26 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L40 AND (L20 OR L21)
L42            33 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L41 OR (L32 OR L33 OR L34 OR
                  L35)
L43            31 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L42 NOT L39
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| | | |
|---|---|---|
| L44 | 30 | SEA FILE=HCAPLUS ABB=ON PLU=ON L43 NOT L12 |
| L45 | 16 | SEA FILE=HCAPLUS ABB=ON PLU=ON L44 AND (?NUCLEOTID? OR DNA OR NUCLEIC OR SEQUENC?) |
| L46 | 9 | SEA FILE=HCAPLUS ABB=ON PLU=ON L45 AND (?CONFORM? OR DUPLEX?) |

9 citations

=> d ibib abs hitstr 1

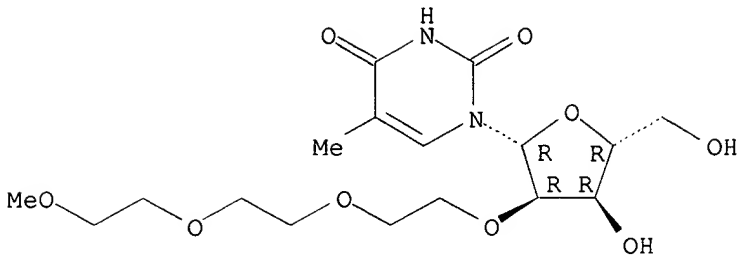
L46 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:446933 HCAPLUS
DOCUMENT NUMBER: 129:184215
TITLE: Correlating Structure and Stability of **DNA Duplexes** with Incorporated 2'-O-Modified RNA Analogs
AUTHOR(S): Tereshko, Valentina; Portmann, Stefan; Tay, Edward C.; Martin, Pierre; Natt, Francois; Altmann, Karl-Heinz; Egli, Martin
CORPORATE SOURCE: Drug Discovery Program and Department of Molecular Pharmacology and Biological Chemistry, Northwestern University Medical School, Chicago, IL, 60611-3008, USA
SOURCE: Biochemistry (1998), 37(30), 10626-10634
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Chem. modified **nucleic** acids are currently being evaluated as potential antisense compds. for therapeutic applications. 2'-O-Ethylene glycol substituted **oligoribonucleotides** are second-generation antisense inhibitors of gene expression with promising features for in vivo use. Relative to **DNA**, they display improved RNA affinity and higher nuclease resistance. Moreover, chimeric **oligonucleotides** with 2'-O-methoxyethyl ribonucleoside wings and a central **DNA** phosphorothioate window have been shown to effectively reduce the growth of tumors in animal models at low doses. Using x-ray crystallog., we have detd. the structures of three **A -form DNA duplexes** contg. the following 2'-O-modified ribothymidine building blocks: 2'-O-methoxyethyl ribo-T, 2'-O-methyl[tri(oxyethyl)] ribo-T, and 2'-O-ethoxymethylene ribo-T. In contrast to 2'-O-ethylene glycol substituents, the presence of a 2'-O-ethoxymethylene group leads to slightly reduced RNA affinity of the corresponding **oligonucleotides**. The three structures allow a qual. rationalization of the differing stabilities of **duplexes** between **oligonucleotides** comprising these types of 2'-O-modified **ribonucleotides** and complementary RNAs. The stabilizing 2'-O-ethylene glycol substituents are **conformationally** preorganized for the **duplex** state. Thus, the presence of one or several ethylene glycol moieties may reduce the **conformational** space of the substituents in an **oligonucleotide** single strand. In addn., most of these preferred **conformations** appear to be compatible with the minor groove topol. in an A-type **duplex**. Factors that contribute to the **conformational** rigidity of the 2'-O-substituents are anomeric and gauche effects, electrostatic interactions between backbone and substituent, and bound water mols.

IT **163760-03-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(**DNA** structures contg.; correlating structure and stability of **DNA duplexes** with incorporated 2'-O-modified RNA analogs)

RN 163760-03-0 HCAPLUS
CN Uridine, 2'-O-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


H
N
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Me
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R
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R
OH
MeO
O
O
O
OH

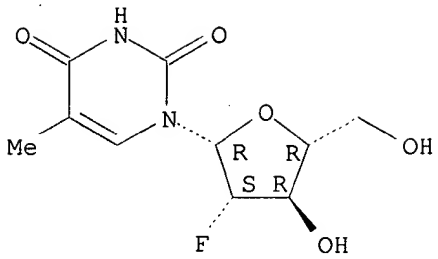
=> d ibib abs hitstr 2

L46 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:391569 HCAPLUS
DOCUMENT NUMBER: 129:145913
TITLE: Crystal structures of B-**DNA** with incorporated 2'-deoxy-2'-fluoro-arabino-furanosyl thymines: implications of **conformational** preorganization for **duplex** stability
AUTHOR(S): Berger, Imre; Tereshko, Valentina; Ikeda, Hisafumi; Marquez, Victor E.; Egli, Martin
CORPORATE SOURCE: Institute for Molecular Biology and Biophysics, ETH-Honggerberg, Zurich, CH-8093, Switz.
SOURCE: Nucleic Acids Research (1998), 26(10), 2473-2480
CODEN: NARHAD; ISSN: 0305-1048
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The fundamental **conformational** states of right-handed double helical **DNA**, the **A**- and **B**-forms, are assocd. with distinct puckers of the sugar moieties. The furanose **conformation** itself is affected by the steric and electronic nature of the ring substituents. For example, a strongly electroneg. substituent at the C2' position, such as in the 2'-deoxy-2'-fluororibofuranosyl analog, will drive the **conformational** equil. toward the C3'-endo type (north). Conversely, the 2'-deoxy-2'-fluoroarabinofuranosyl modification with opposite stereochem. at C2' appears to have a preference for a C2'-endo type pucker (south). Incorporation of 2'-fluoroarabinofuranosyl thymines was previously shown to enhance the thermodn. stability of B-**DNA duplexes**. We have detd. the crystal structures of the B-**DNA** dodecamer **duplexes** [d(CGCGAASSCGCG)]2 and [d(CGCGAASTCGCG)]2 with incorporated 2'-deoxy-2'-fluoroarabinofuranosyl thymines S (south) at 1.55 .ANG. resoln. In the crystal structures, all S residues adopt an O4'-endo **conformation** (east), well compatible with an overall **B-form duplex** geometry. In addn. to the increased rigidity of S nucleosides, a clathrate-like ordered water structure around the 2'-fluorines may account for the obsd. larger thermodn. stability of **DNA duplexes** contg. 2'-deoxy-2'-fluoroarabino thymidines.

IT **69256-17-3**
RL: PRP (Properties)
(crystal structures of B-**DNA** with incorporated 2'-deoxy-2'-fluoro-arabino-furanosyl thymines and implications of **conformational** preorganization for **duplex** stability)
RN 69256-17-3 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-2-fluoro-.beta.-D-arabinofuranosyl)-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.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S
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F
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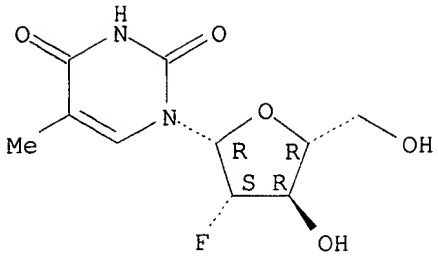
=> d ibib abs hitstr 3

L46 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:318623 HCAPLUS
DOCUMENT NUMBER: 129:50988
TITLE: The effect of two antipodal fluorine-induced sugar puckers on the **conformation** and stability of the Dickerson-Drew dodecamer **duplex** [d(CGCGAATTCGCG)]2
AUTHOR(S): Ikeda, Hisafumi; Fernandez, Raul; Wilk, Andrzej; Barchi, Joseph J., Jr.; Huang, Xiaolin; Marquez, Victor E.
CORPORATE SOURCE: Laboratory of Medicinal Chemistry, Division of Basic Sciences, National Cancer Institute, National Institutes of Health, Food and Drug Administration, Bethesda, MD, 20892, USA
SOURCE: Nucleic Acids Research (1998), 26(9), 2237-2244
CODEN: NARHAD; ISSN: 0305-1048
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB UV thermal melting studies, CD and NMR spectroscopies were employed to assess the contribution of antipodal sugar **conformations** on the stability of the canonical B-**DNA conformation** of the Dickerson-Drew dodecamer **duplex** {[d(CGCGAATTCGCG)]2, (ODN 1)}. Different **oligodeoxynucleotide** versions of ODN 1 were synthesized with modified thymidine units favoring distinct sugar **conformations** by using a 3'-endo (north) 2'-fluoro-2'-deoxyribofuranosyl thymine (1) or a 2'-endo (south) 2'-fluoro-2'-deoxyarabinofuranosyl thymine (2). The results showed that two south thymidines greatly stabilized the double helix, whereas two north thymidines destabilized it by inducing a more A-like **conformation** in the middle of the **duplex**. Use of combinations of north and south thymidine **conformers** in the same oligo destabilized the double helix even further, but without inducing a **conformational** change. The crit. length for establishing a detectable A-like **conformation** in the middle of **a B-DNA** ODN appears to be 4 bp. Our results suggest that manipulation of the **conformation** of **DNA** in a **sequence**-independent manner is possible.

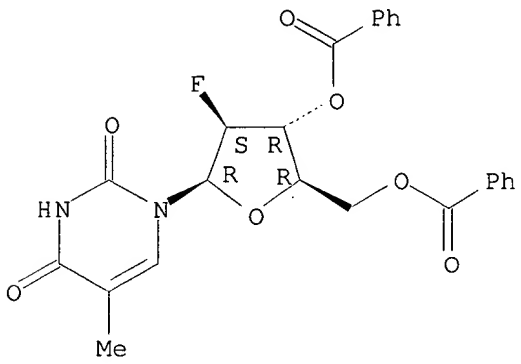
IT **69256-17-3P 97614-47-6P 122799-38-6P 133324-02-4P 144822-48-0P 182700-06-7P 208193-47-9P 208193-48-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 3'-endo (north) 2'-fluoro-2'-deoxyribofuranosyl thymine and 2'-endo (south) 2'-fluoro-2'-deoxyarabinofuranosyl thymine **conformers**)
RN 69256-17-3 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-2-fluoro-.beta.-D-arabinofuranosyl)-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



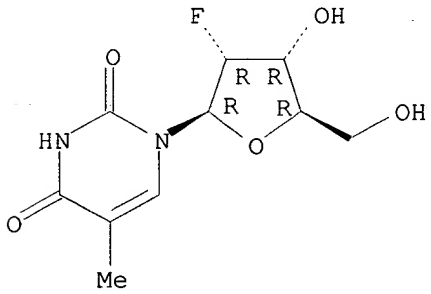
RN 97614-47-6 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1-(3,5-di-O-benzoyl-2-deoxy-2-fluoro-.beta.-D-arabinofuranosyl)-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



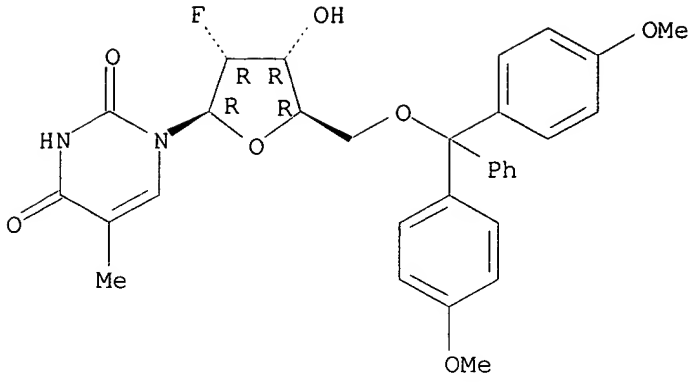
RN 122799-38-6 HCAPLUS
CN Uridine, 2'-deoxy-2'-fluoro-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



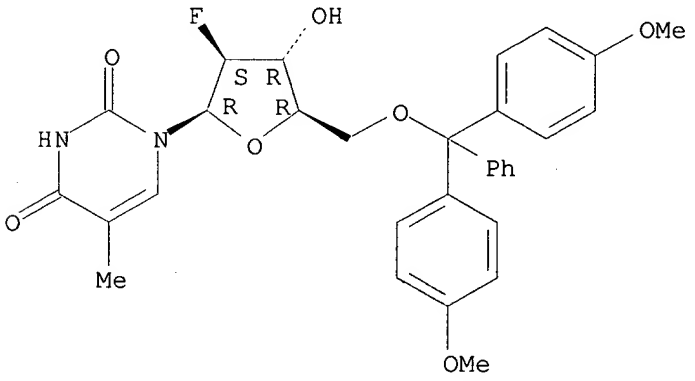
RN 133324-02-4 HCAPLUS
CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-2'-fluoro-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



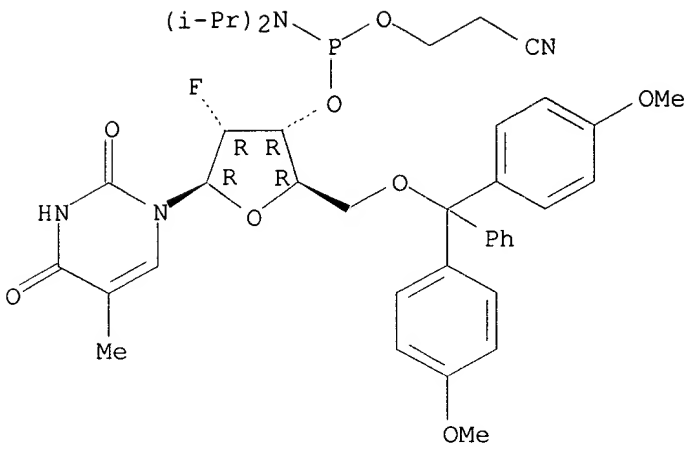

RN 144822-48-0 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-2-fluoro-.beta.-D-arabinofuranosyl]-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



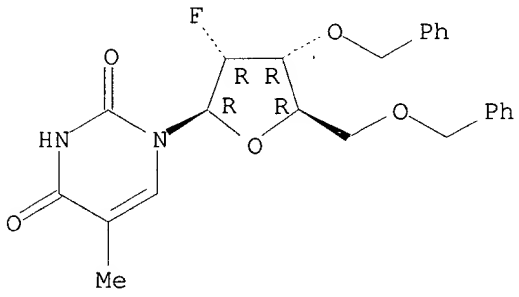

RN 182700-06-7 HCAPLUS
CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-2'-fluoro-5-methyl-, 3'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



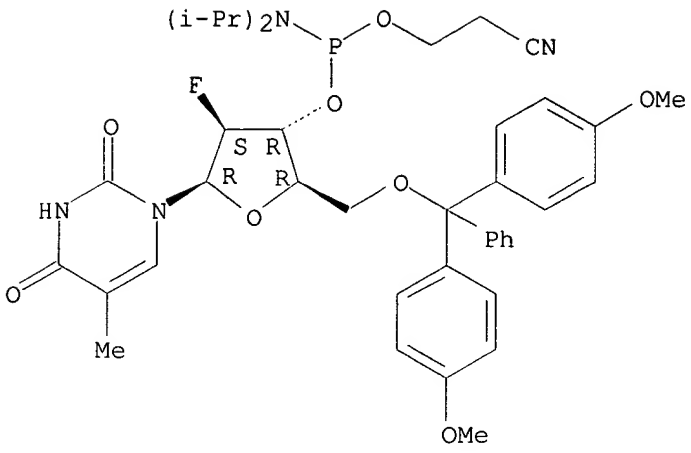

RN 208193-47-9 HCAPLUS
CN Uridine, 2'-deoxy-2'-fluoro-5-methyl-3',5'-bis-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




RN 208193-48-0 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1-[5-O-[bis(4-methoxyphenyl)phenylmethyl]-3-O-[[bis(1-methylethyl)amino](2-cyanoethoxy)phosphino]-2-deoxy-2-fluoro-.beta.-D-arabinofuranosyl]-5-methyl- (9CI) (CA INDEX NAME)

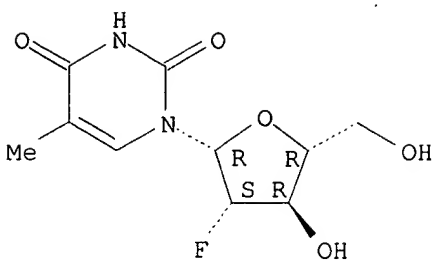
Absolute stereochemistry.


(i-Pr)2N
P
O
CN
F
O
OMe
O
S R
R R
HN
N
O
O
Ph
Me
OMe

=> d ibib abs hitstr 4

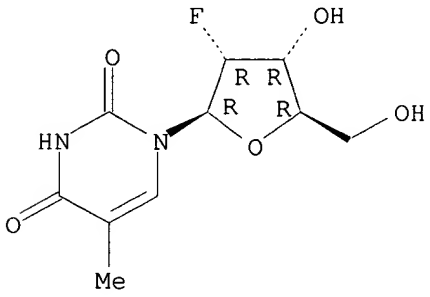
L46 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:35923 HCAPLUS
DOCUMENT NUMBER: 126:196486
TITLE: The molecular modeling calculations of **DNA**:RNA double helical structures with modified **oligodeoxynucleotides** and the correlation of their antisense activities
AUTHOR(S): Ren, Wu Yun; Watanabe, Kyoichi A.
CORPORATE SOURCE: Sloan-Kettering Div. Grad. Sch. Med. Sch., Cornell Univ., New York, NY, 10021, USA
SOURCE: Korean Journal of Medicinal Chemistry (1996), 6(2), 166-182
CODEN: KJMCE7; ISSN: 1225-0058
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We present computer simulations for three dimensional structures with an anal. of the no. of selected hydrogen bonds, mol. similarity, and nonbonded energies. The studies were carried out on six modified **DNA**:natural RNA hybrids (with modified base, sugar and/or phosphate backbones). We have modeled the three dimensional structural illustrations and provided an anal. of the no. of selected H-bonds, minimization and dynamic energy, and calcd. mol. vols. The data indicate that (1) the phosphorothioate backbone of **oligodeoxynucleotides** increased the stability of **DNA**:RNA hybrids, and that **A -form** was the preferred **conformation**. (2) C5-propyne deoxyuridine contg. oligomers with phosphorothioate backbones formed the most stable hybrids. (3) While replacement of the thymidine residues in the oligomers with 2'-O-allyl-5-methyluridine increased the stability of the hybrids, antisense activity was diminished. These findings suggest that helical stability was assocd. with alignment of O-allyl group on the outer rim of the double helix and this alignment also prevented RNase H recognition of the hybrids as substrates. (4) 2'-Fluoro substitutes in either .alpha. or .beta. oligomer configurations resulted in increased electrostatic energy within each of the hybrids;. (5) Finally, we noted that the random (natural) **sequence** of the 2'-fluoro substituted oligomers showed reduced Lennard-Jones energy (Van der Waals force) compared to the other **sequences** that were studied.
IT **69256-17-3 122799-38-6**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(mol. modeling calcns. of **DNA**-RNA double helical structures with modified **oligodeoxynucleotides** and the correlation of their antisense activities)
RN 69256-17-3 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1-(2-deoxy-2-fluoro-.beta.-D-arabinofuranosyl)-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 122799-38-6 HCAPLUS
CN Uridine, 2'-deoxy-2'-fluoro-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



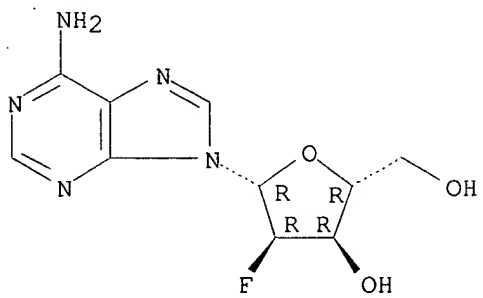
=> d ibib abs hitstr 5

L46 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1993:575361 HCAPLUS
DOCUMENT NUMBER: 119:175361
TITLE: **Oligodeoxynucleotides** containing 2'-O-modified adenosine: Synthesis and effects on stability of **DNA**:RNA **duplexes**
AUTHOR(S): Lesnik, Elena A.; Guinosso, Charles J.; Kawasaki, Andrew M.; Sasmor, Henri; Zounes, Maryann; Cummins, Lendell L.; Ecker, David J.; Cook, P. Dan; Freier, Susan M.
CORPORATE SOURCE: Dep. Mol., Cell. Struct. Biol., ISIS Pharm., Carlsbad, CA, 92008, USA
SOURCE: Biochemistry (1993), 32(30), 7832-8
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Hybridization thermodn. were compared for **oligonucleotide sequences** contg. 2'-fluoro dA, 2'-O-Me A, 2'-O-Et A, 2'-O-Pr A, 2'-O-Bu A, 2'-O-pentyl A, 2'-O-nonyl A, 2'-O-allyl A, and 2'-O-benzyl A in place of deoxyadenosine. Although the effect of 2'-modified adenosine on **duplex** stability is **sequence** dependent, a clear trend is apparent. For six **sequences** contg. a few 2'-modified adenosines in a background of unmodified **deoxynucleotides**, the av. .DELTA.TM per substitution ranged from +1.3.degree. for 2'-fluoro dA to -2.0.degree. for 2'-O-nonyl A. For the 2'-O-alkyl series, the av. .DELTA.TM per substitution correlates well with size of the substituent; the order of stability is 2'-O-Me A > 2'-O-Et A > 2'-O-Pr A > 2'-O-Bu A > 2'-O-pentyl A > 2'-O-nonyl A. This correlation also extends to 2'-fluoro dA, 2'-O-allyl A, and 2'-O-benzyl A if chain length is measured by no. of carbon atoms. When examd. in the background of 2'-O-Me **ribonucleotides**, all 2'-modified adenosines with a substituent no larger than 2'-O-pentyl stabilized the **duplex** nearly 2.degree. per substitution compared to unmodified dA. These thermodn. results and CD spectra of modified and unmodified hybrids support a model of **DNA**:RNA hybrids in which the geometry is between that of **B -form** and **A-form**.

IT **64183-27-3**, 2'-Fluoro-2'-deoxyadenosine
RL: BIOL (Biological study)
(**oligodeoxynucleotides** contg., prepn. and **DNA**:RNA **duplex** stability of)
RN 64183-27-3 HCAPLUS
CN Adenosine, 2'-deoxy-2'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

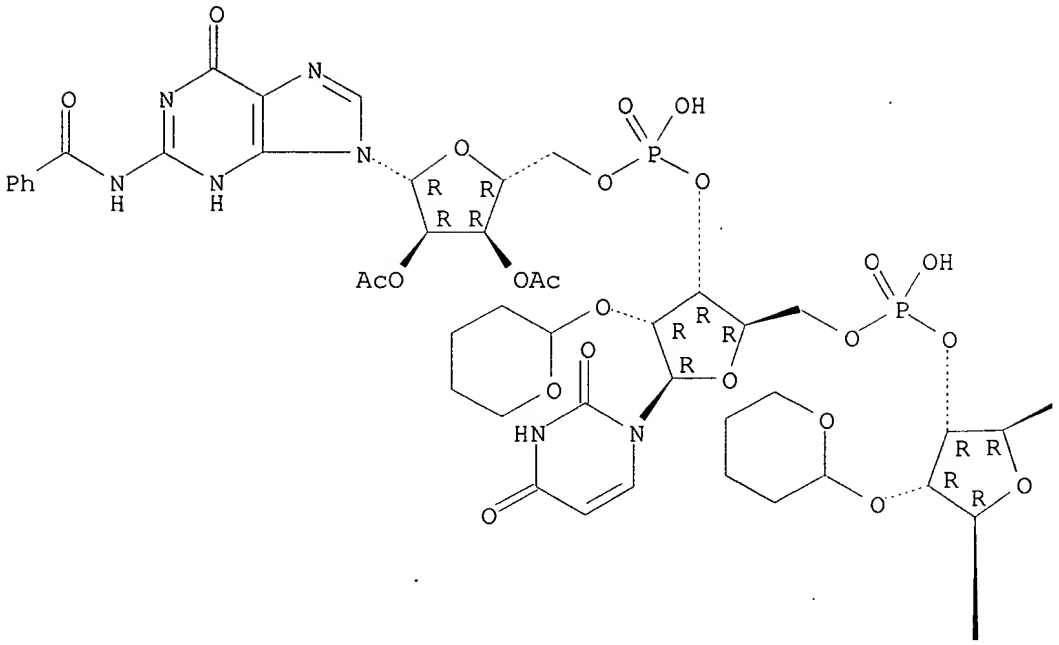


=> d ibib abs hitstr 6

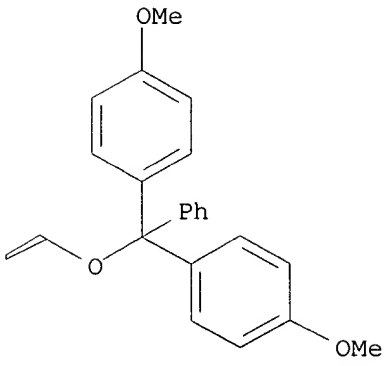
L46 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1991:626347 HCAPLUS
DOCUMENT NUMBER: 115:226347
TITLE: Thermodynamic and structural properties of pentamer **DNA**.cntdot.**DNA**, RNA.cntdot.RNA and **DNA**.cntdot.RNA **duplexes** of identical **sequence**
AUTHOR(S): Hall, Kathleen B.; McLaughlin, Larry W.
CORPORATE SOURCE: Sch. Med., Washington Univ., St. Louis, MO, 63110, USA
SOURCE: Biochemistry (1991), 30(44), 10606-13
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Four pentamers with the general **sequence** 5'CU(T)GU(T)G/5'CACAG have been prepd. by chem. synthesis in order to generate **duplex** structures with common **sequences**. The four **duplexes** studied include the **DNA**.cntdot.**DNA duplex** (5'dCACAG/5'dCTGTG) and the RNA.cntdot.RNA **duplex** (5'rCUGUG/5'rCACAG) as well as the two corresponding **DNA** .cntdot.RNA heteroduplexes (5'rCUGUG/5'dCACAG and 5'rCACAG/5'dCTGTG). The measured entropy, enthalpy, and free energy changes upon melting are reported for each pentamer and compared to the predicted values where possible. Results show that the two **DNA**.cntdot.RNA heteroduplexes are destabilized (.DELTA.G.degree.25 = 4.2 kcal/mol) relative to either the **DNA**.cntdot.**DNA duplex** (.DELTA.G.degree.25 = -4.8 kcal/mol) or the RNA.cntdot.RNA **duplex** (.DELTA.G.degree.25 = -5.8 kcal/mol). CD spectra indicate that the RNA and the two heteroduplexes adopt an **A-form conformation**, while the **DNA conformation** is **B-form**. Imino proton NMR spectra also show that the heteroduplex structures resemble the RNA.cntdot.RNA **duplex**.
IT **136658-84-9**
RL: RCT (Reactant)
(reaction of, with chlorophenylbisbenzotriazolylphosphate)
RN 136658-84-9 HCAPLUS
CN Guanosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-N-(4-methoxybenzoyl)-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'.fwdarw.5')-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-N-benzoyl-, 2',3'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

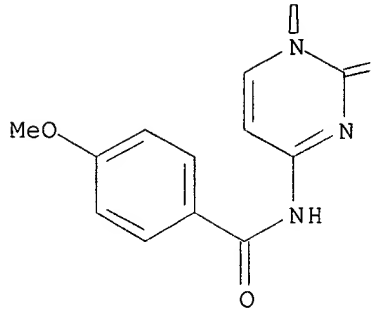
PAGE 1-A



PAGE 1-B



PAGE 2-A

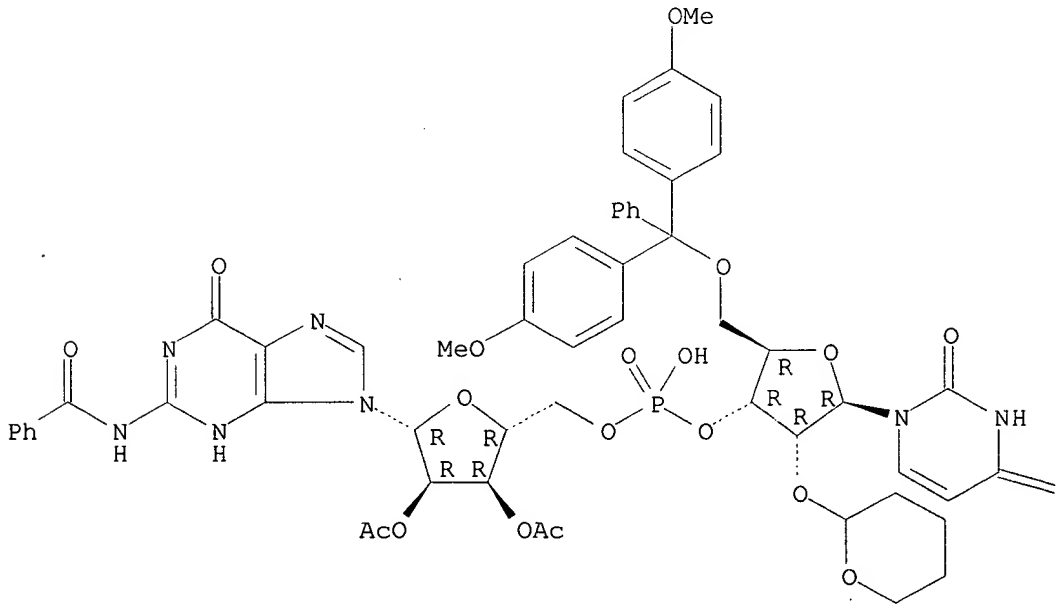


PAGE 2-B

IT **136631-61-3**
RL: RCT (Reactant)
(reaction of, with **nucleotide** trimer hydroxytriazoyl deriv.)
RN 136631-61-3 HCAPLUS
CN Guanosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-O-(tetrahydro-2H-pyran-2-yl)uridylyl-(3'.fwdarw.5')-N-benzoyl-, 2',3'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



=/=o

=> d ibib abs hitstr 7

L46 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1982:610742 HCAPLUS
DOCUMENT NUMBER: 97:210742
TITLE: Specific interaction of netropsin, distamycin-3 and analogs with I.cntdot.C **duplexes**: reversion towards the **B form** of 2'-deoxy-.cntdot.2'-deoxy-2'-fluoro- hybrid **duplexes** upon specific interaction with netropsin, distamycin-3 and analogs
AUTHOR(S): Marck, Christian; Kakiuchi, Nobuko; Guschlbauer, Wilhelm
CORPORATE SOURCE: Dep. Biol., Cent. Etud. Nucl. Saclay, Gif-sur-Yvette, F-91191, Fr.
SOURCE: Nucleic Acids Res. (1982), 10(19), 6147-61
CODEN: NARHAD; ISSN: 0305-1048
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Binding of the **B-form**-specific ligands netropsin (I) and distamycin-3, -4, and -5 was used to monitor the presence and(or) the inducibility of **a B**-type structure in various poly(I).cntdot.poly(C) double-stranded polymers with deoxyribose, ribose, or 2'-deoxy-2'-fluororibose as the sugar on either strand. The efficiency of binding was followed by CD and further evaluated by the increase in melting temp. of the complexes. The efficient binding of I and distamycins to the hybrid polymer (2'-fluoro-dI)n.cntdot.(dC)n demonstrated that the Fl--carrying strand may undergo a **A**-to-**B**-type transition, reflecting a change of the 2'-deoxy-2'-fluororibose from the 3'-endo to the 1'-exo or 2'-endo pucker. The less efficient binding of the same ligands to the reverse factor (dI)n.cntdot.(2'-deoxy-dC)n showed that the geometry of the pyrimidine strand is the most crit. factor for specific interaction. Taking into account recent findings about the regular hydration in the minor groove of the B-type dodecamer dCGCGAATTCGCG in the solid state, the different binding modes obsd. between the different polymers and antibiotics are explained by differences in their possibilities of hydration. Binding of I to a double-stranded **deoxynucleotide** polymer is interpreted as a local replacement of water mols. by I in the minor groove hydration network, which is typical of the **B-form**.
IT **80145-10-4 80155-11-9**
RL: BIOL (Biological study)
(**conformational** flexibility of, distamycin and netropsin binding in relation to)
RN 80145-10-4 HCAPLUS
CN 5'-Inosinic acid, 2'-deoxy-2'-fluoro-, homopolymer, complex with 2'-deoxy-5'-cytidylic acid homopolymer (1:1) (9CI) (CA INDEX NAME)

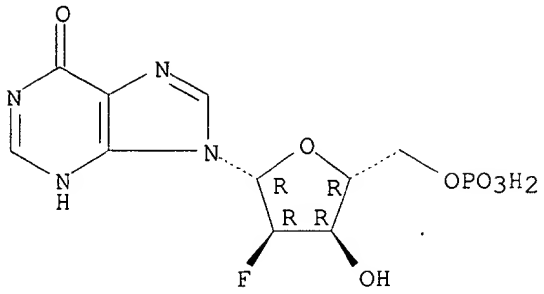
CM 1

CRN 68777-95-7
CMF (C10 H12 F N4 O7 P)x
CCI PMS

CM 2

CRN 68777-94-6
CMF C10 H12 F N4 O7 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



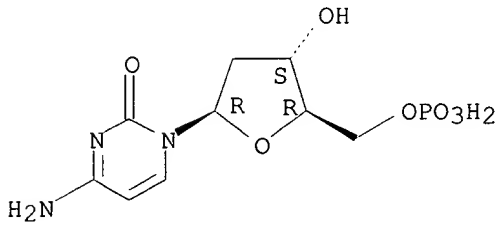

CM 3

CRN 25609-92-1
CMF (C9 H14 N3 O7 P)x
CCI PMS.

CM 4

CRN 1032-65-1
CMF C9 H14 N3 O7 P
CDES 5:B-D-ERYTHRO

Absolute stereochemistry.




RN 80155-11-9 HCAPLUS
CN 5'-Inosinic acid, 2'-deoxy-, homopolymer, complex with 2'-deoxy-2'-fluoro-5'-cytidylic acid homopolymer (1:1) (9CI) (CA INDEX NAME)

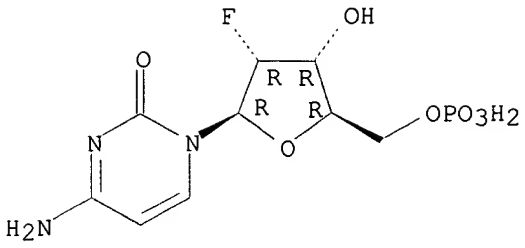
CM 1

CRN 63541-63-9
CMF (C9 H13 F N3 O7 P)x
CCI PMS

CM 2

CRN 63541-62-8
CMF C9 H13 F N3 O7 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



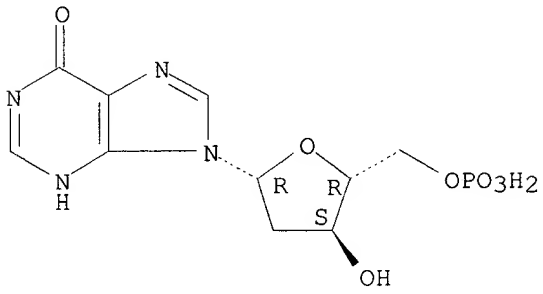

CM 3

CRN 27732-54-3
CMF (C10 H13 N4 O7 P)x
CCI PMS

CM 4

CRN 3393-18-8
CMF C10 H13 N4 O7 P
CDES 5:B-D-ERYTHRO

Absolute stereochemistry.



=> d ibib abs hitstr 8

L46 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1982:195289 HCAPLUS
DOCUMENT NUMBER: 96:195289
TITLE: Differential stabilization by netropsin of inducible B-like **conformations** in deoxyribo-, ribo- and 2'-deoxy-2'-fluororibo-adenosine containing **duplexes** of (dA)n.cntdot.(dT)n and (dA)n.cntdot.(dU)n
AUTHOR(S): Zimmer, Christoph; Kakiuchi, Nobuko; Guschlbauer, Wilhelm
CORPORATE SOURCE: Dep. Biol., CEN Saclay, Gif-sur-Yvette, F-91191, Fr.
SOURCE: Nucleic Acids Res. (1982), 10(5), 1721-32
CODEN: NARHAD; ISSN: 0305-1048
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Six **polynucleotide duplexes** contg. poly(dA), poly(A), or poly-2'-deoxy-2'-fluoroadenylic acid (polydAfl) in 1 strand, and poly(dU) or poly(dT) in the other strand were studied by CD, ionic strength-dependence of melting temps., and binding of the **DNA** -specific antibiotic netropsin. CD spectra of (dA)n.cntdot.(dT)n and (dA)n.cntdot.(dU)n indicated the presence of the **B-form** of **DNA**, whereas those of (dAfl)n.cntdot.(dT)n and (A)n.cntdot.(dT)n (and the corresponding (dU)n hybrids) indicated the presence of the **A-form**. The (dAfl)n.cntdot.(dT)n and (dAfl)n.cntdot.(dU)n bound netropsin only slightly less than the (dA)n-contg. **duplexes**, whereas replacement by (A)n decreased netropsin binding to a large degree. Since netropsin requires B-**DNA** for binding, the **A** to **B** transition is facilitated in the case of F substitution in the sugar moiety, whereas the 2'-OH group greatly limits this **conformational** change.
IT **68246-13-9 81795-97-3**
RL: PRP (Properties)
(**conformation** of, CD and netropsin binding in relation to)
RN 68246-13-9 HCAPLUS
CN 5'-Adenylic acid, 2'-deoxy-2'-fluoro-, homopolymer, complex with 5'-uridylic acid homopolymer (1:1) (9CI) (CA INDEX NAME)

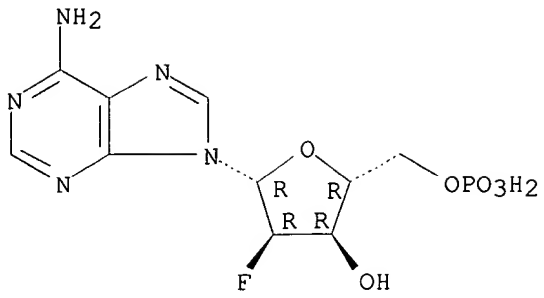
CM 1

CRN 68245-92-1
CMF (C10 H13 F N5 O6 P)x
CCI PMS

CM 2

CRN 68245-91-0
CMF C10 H13 F N5 O6 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



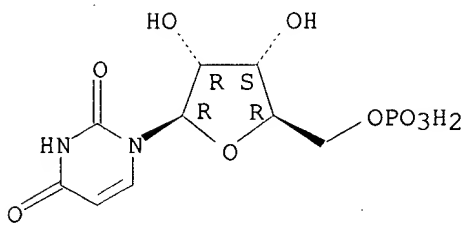
CM 3

CRN 27416-86-0
CMF (C9 H13 N2 O9 P)x
CCI PMS

CM 4

CRN 58-97-9
CMF C9 H13 N2 O9 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



RN 81795-97-3 HCAPLUS
CN 5'-Adenylic acid, 2'-deoxy-2'-fluoro-, homopolymer, complex with 5'-thymidylic acid homopolymer (1:1) (9CI) (CA INDEX NAME)

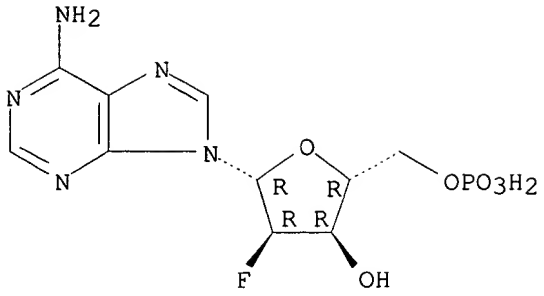
CM 1

CRN 68245-92-1
CMF (C10 H13 F N5 O6 P)x
CCI PMS

CM 2

CRN 68245-91-0
CMF C10 H13 F N5 O6 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



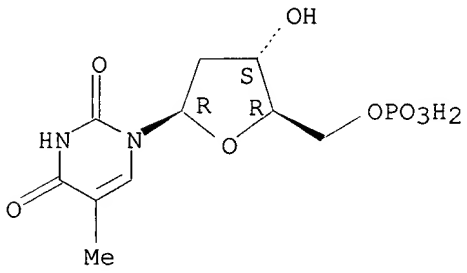

CM 3

CRN 25086-81-1
CMF (C10 H15 N2 O8 P)x
CCI PMS

CM 4

CRN 365-07-1
CMF C10 H15 N2 O8 P
CDES 5:B-D-ERYTHRO

Absolute stereochemistry.



=> d ibib abs hitstr 9

L46 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:151689 HCAPLUS
DOCUMENT NUMBER: 86:151689
TITLE: Structural studies of synthetic **polynucleotides** by polarographic techniques
AUTHOR(S): Janik, Borek; Sommer, Ronald G.
CORPORATE SOURCE: Res. Prod., Miles Lab., Inc., Elkhart, Indiana, USA
SOURCE: Bioelectrochem. Bioenerg. (1976), 3(3-4), 622-33
CODEN: BEBEBP
DOCUMENT TYPE: Journal
LANGUAGE: English

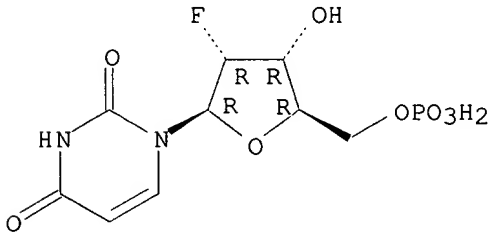
AB Correlation of polarog. parameters with mol.-wt. characteristics were demonstrated for **polynucleotides** which are polarog. nonreducible, poly(U) and poly(dUfl) [poly(fluorodeoxyuridylic acid)], and reducible, poly(A). In the 1st case, a function of the differential capacitance K was found proportional to the sedimentation coeff. of the **polynucleotide**. Close similarity of such proportionality indicated that substitution of the 2'-OH group in poly(U) by the 2'-F group in poly(dUfl) has only a neglible effect on adsorption properties. In the case of poly(A), a relation was demonstrated between redn. currents and the chain length (or mol. wt.) of the **polynucleotide**. Agreement of the exptl. relations with theor. predictions supports the idea of the impermeable coil model for diffusing poly(A) mols. The variation of current with pH for poly(A) at acidic pH assumed **a form** which essentially depended on how the pH of the sample was reached. Interpreting the current variations in terms of availability of redn. sites and considering the temp.-absorbance profiles, CD, UV titrn. curves, and reactivity with HCHO, 3 forms of poly(A) at acid pH are postulated, i.e. intermediate, frozen, and tightly packed forms, all of these forms being **conformationally** distinct.

IT **36087-76-0**
RL: PRP (Properties)
(**conformation** of, polarog. in relation to)
RN 36087-76-0 HCAPLUS
CN 5'-Uridylic acid, 2'-deoxy-2'-fluoro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 50270-97-8
CMF C9 H12 F N2 O8 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



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The answer numbers requested are not in the answer set.
ENTER ANSWER NUMBER OR RANGE (1):end
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STR Search

KRISHNAN 09/970,971

Same STR as L39

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L13               STR
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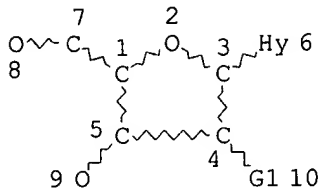


O~Cy
@11 12

O~G2~Ak~O
@13 14 15 16

Ak~O
@17 @18

Ak~O~N
@20 21 @22

O~G3~Ak~O
@23 24 25 26

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REP G2=(1-10) 17-13 18-15
REP G3=(1-10) 20-23 22-25
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GGCAT   IS LIN  SAT  AT  15
GGCAT   IS LIN  SAT  AT  17
GGCAT   IS LIN  SAT  AT  20
GGCAT   IS LIN  SAT  AT  25
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M4 C  AT   6
ECOUNT  IS X10 C  AT  15
ECOUNT  IS M2-X10 C  AT  17
ECOUNT  IS M2-X10 C  AT  20
ECOUNT  IS X10 C  AT  25

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  25

STEREO ATTRIBUTES: NONE
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L17           858 SEA FILE=REGISTRY ABB=ON  PLU=ON  L16 AND NCNC3/ES AND
                  NCNC2-NCNC3/ES
L18           858 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 AND P/ELS
L19          4227 SEA FILE=REGISTRY ABB=ON  PLU=ON  L16 NOT L18
L20           222 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L18
L21          2311 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19
L29        441158 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ?CONFORMATION? OR ?GEOMETRY?
                  OR ENDO OR ?CONFORMER?
L30         19435 SEA FILE=HCAPLUS ABB=ON  PLU=ON  A"-"FORM
L31          2857 SEA FILE=HCAPLUS ABB=ON  PLU=ON  B"-"FORM
L32             3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 AND L20
L33             7 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 AND L21
L34             4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L31 AND L20
L35             5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L31 AND L21
L36           120 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L29 AND (L20 OR L21)
L37            39 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L36 AND ENDO
L38             2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L32 OR L34) AND (L33 OR L35)

L39             2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L38 NOT L12
L40        182405 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "A AND B"
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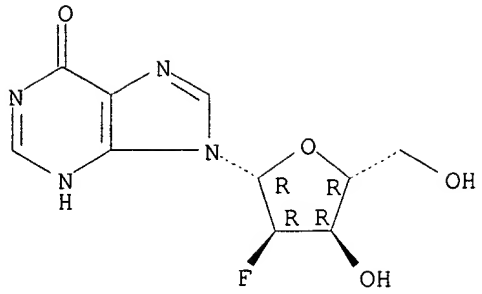
| L42 | 33 | SEA FILE=HCAPLUS ABB=ON PLU=ON L41 OR (L32 OR L33 OR L34 OR L35) |
| L43 | 31 | SEA FILE=HCAPLUS ABB=ON PLU=ON L42 NOT L39 |
| L47 | 22 | SEA FILE=HCAPLUS ABB=ON PLU=ON L37 AND (?NUCLEOTID? OR DNA OR NUCLEIC OR SEQUENC? OR DUPLEX) |
| L48 | 18 | SEA FILE=HCAPLUS ABB=ON PLU=ON L47 NOT L43 |
| L49 | 4 | SEA FILE=HCAPLUS ABB=ON PLU=ON L48 AND OLIGONUC? |

4 cites

=> d ibib abs hitstr 1

L49 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:473246 HCAPLUS
DOCUMENT NUMBER: 136:33484
TITLE: The occurrence of the syn-C3' **endo** **conformation** and the distorted backbone **conformations** for C4'-C5' and P-O5' in oligo and **polynucleotides**
AUTHOR(S): Vasudevan, Sanjay S.; Sundaralingam, Muttaiya
CORPORATE SOURCE: The Biological Macromolecular Structure Center, Departments of Chemistry and Biochemistry, The Ohio State Biochemistry Program, Ohio State University, Columbus, OH, 43210, USA
SOURCE: Journal of Biomolecular Structure & Dynamics (2001), 18(6), 824-831
CODEN: JBSDD6; ISSN: 0739-1102
PUBLISHER: Adenine Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The nucleoside constituents of **nucleic** acids prefer the anti **conformation** (1). When the sugar pucker is taken into account the nucleosides prefer the C2' **endo**-anti **conformation**. Of the nearly 300 nucleosides known, about 250 are in the anti **conformation** and 50 are in the syn-**conformation**, i.e., anti to syn **conformation** is 5:1. The **nucleotide** building blocks of **nucleic** acids show the same trend as nucleosides. Both the deoxy-guanosine and ribo-guanosine residues in nucleosides and **nucleotides** prefer the syn-C2' **endo** **conformation** with an intra-mol. hydrogen bond (for nucleosides) between the O5'-H and the N3 of the base and, a few syn-C3' **endo** **conformations** are also obsd. Evidence is presented for the occurrence of the C3' **endo**-syn **conformation** for guanines in mis-paired double helical right-handed structures with the distorted sugar phosphate C4'-C5' and P-O5' bonds resp., from g+ (gg) and g- to trans. Evidence is also provided for guanosine **nucleotides** in left-handed double-helical (Z-**DNA**) oligo and **polynucleotides** which has the same syn-C3' **endo** **conformation** and the distorted backbone sugar-phosphate bonds (C4'-C5' and P-O5') as in the earlier right-handed case.
IT **78102-02-0**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(occurrence of the syn-C3' **endo** **conformation** and the distorted backbone **conformations** for C4'-C5' and P-O5' in oligo and **polynucleotides**)
RN 78102-02-0 HCAPLUS
CN Inosine, 2'-deoxy-2'-fluoro-, monohydrate (9CI) (CA INDEX NAME)

Absolute stereochemistry.




● $H_2O$

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 2

L49 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:98585 HCAPLUS
DOCUMENT NUMBER: 132:137670
TITLE: RNA targeted 2'-modified **oligonucleotides** that are **conformationally** pre-organized
INVENTOR(S): Manoharan, Muthiah; Mohan, Venkatraman; Boswell, Herb
PATENT ASSIGNEE(S): Isis Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000006590 | A1 | 20000210 | WO 1999-US16541 | 19990721 |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 6271358 | B1 | 20010807 | US 1998-123108 | 19980727 |
| AU 9951213 | A1 | 20000221 | AU 1999-51213 | 19990721 |
| EP 1100809 | A1 | 20010523 | EP 1999-935814 | 19990721 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |

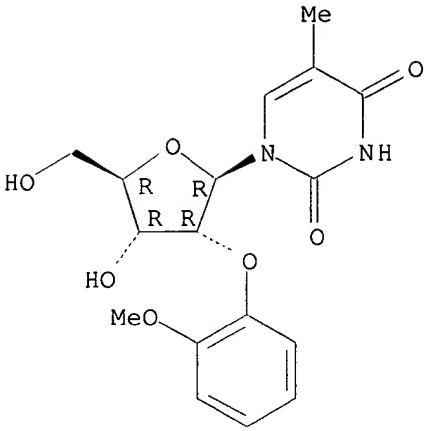
PRIORITY APPLN. INFO.: US 1998-123108 A1 19980727
WO 1999-US16541 W 19990721

AB 2'-O-modified ribosyl nucleosides and modified **oligonucleotides** contg. such **nucleotides** are disclosed. **Oligonucleotides** are disclosed that have increased binding affinity to hepatitis C virus as shown by mol. modeling expts. The 2'-O-modified nucleosides of the invention include ring structures that position the sugar moiety of the nucleosides preferentially in 3' **endo** geometries.

IT **256420-89-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(RNA targeted modified **oligonucleotides** that are **conformationally** pre-organized)

RN 256420-89-0 HCAPLUS
CN Uridine, 2'-O-(2-methoxyphenyl)-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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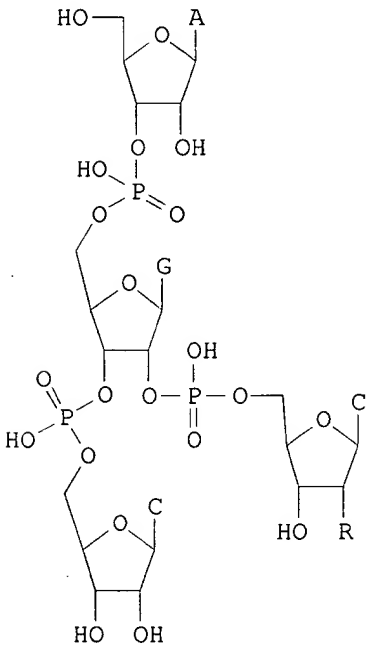
L49 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2002 ACS
IC ICM C07H021-02
ICS C07H021-04; C07H019-04; C07H019-20; C07H019-048; C07H019-10; C07H019-167; C07H019-173; C07H019-06; C07H019-09
CC 33-10 (Carbohydrates)
Section cross-reference(s): 1
ST RNA **oligonucleotide** binding affinity mol modeling prepn; hepatitis C antiviral mol modeling **oligonucleotide** prepn; antisense **oligodeoxyribonucleotide** prepn binding affinity mol modeling
IT Antiviral agents
Molecular modeling
(RNA targeted modified **oligonucleotides** that are **conformationally** pre-organized)
IT Antisense **oligonucleotides**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(RNA targeted modified **oligonucleotides** that are **conformationally** pre-organized)
IT 155752-74-2P 156658-10-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(RNA targeted modified **oligonucleotides** that are **conformationally** pre-organized)
IT 90-05-1, 2-Methoxyphenol 22423-26-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(RNA targeted modified **oligonucleotides** that are **conformationally** pre-organized)
IT **256420-89-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(RNA targeted modified **oligonucleotides** that are **conformationally** pre-organized)

=> d ibib abs hitstr 3

L49 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1991:656476 HCAPLUS
DOCUMENT NUMBER: 115:256476
TITLE: Synthesis of tetrameric branched RNA-**DNA** conjugate and branched-RNA analog and their comparative **conformational** studies by 500 MHz NMR spectroscopy
AUTHOR(S): Foldesi, Andras; Agback, Peter; Glemarec, Corin; Chattopadhyaya, Jyoti
CORPORATE SOURCE: Biomed. Cent., Univ. Uppsala, Uppsala, S-751 23, Swed.
SOURCE: Tetrahedron (1991), 47(34), 7135-56
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



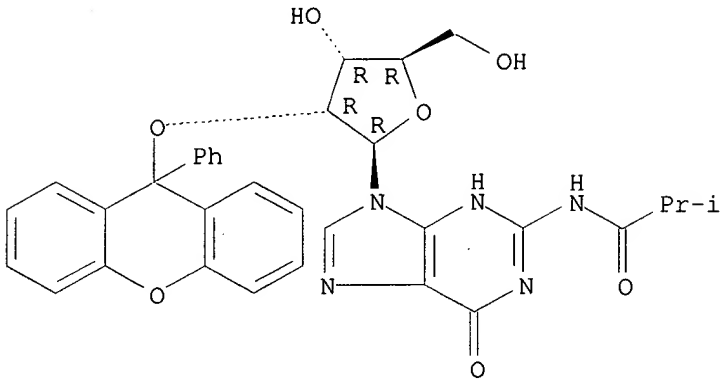
I

AB The unambiguous synthesis of pure tetrameric branched **oligonucleotides** I found naturally in gram-neg. bacterium Stigmatella aurantiaca, and corresponding branched RNA analog. The **conformational** features of branched tetramers I have been elucidated and compared by assessing temp.- and concn.-dependent 1H and 31P chem. shifts, (C2'-exo and C3'-**endo**).dblarw.(C2'-**endo**, C3'-exo) equil., and equil. amongst staggered .gamma. and .beta. rotamers using various 2D homo- and heteronuclear correlation, NOSEY and ROSEY expts. by 500 MHz NMR spectroscopy.

IT **137272-75-4**
RL: RCT (Reactant)
(coupling of, with a **nucleotide**)

RN 137272-75-4 HCAPLUS
CN Guanosine, N-(2-methyl-1-oxopropyl)-2'-O-(9-phenyl-9H-xanthen-9-yl)- (9CI) (CA INDEX NAME)

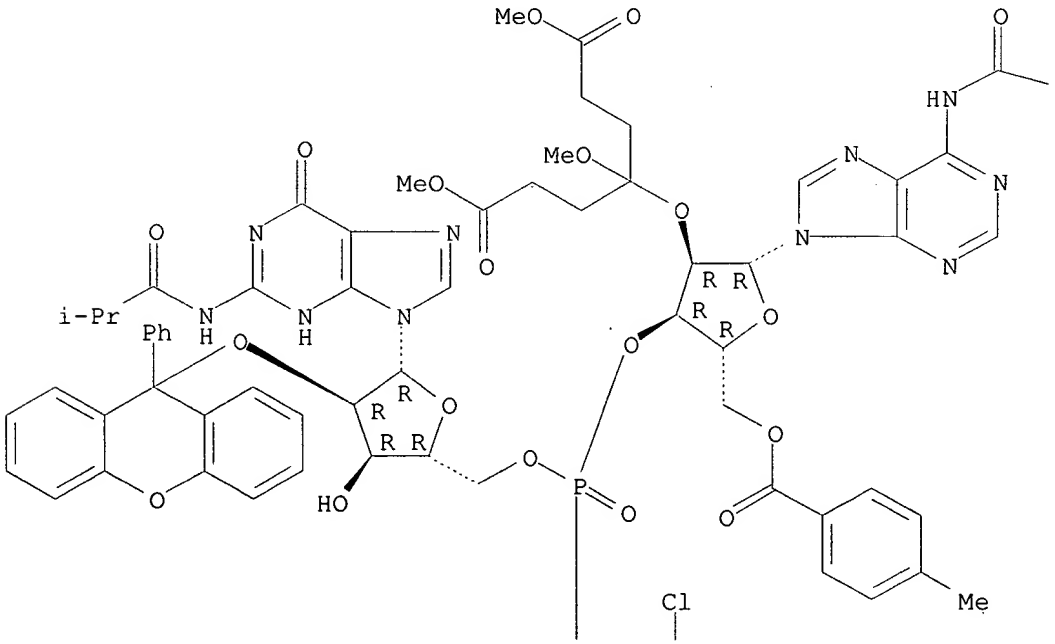
Absolute stereochemistry.



IT **137272-76-5P 137272-80-1P 137335-94-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in synthesis of branched **oligoribonucleotides**)
RN 137272-76-5 HCAPLUS
CN Guanosine, N-benzoyl-P-(2-chlorophenyl)-2'-O-[1,4-dimethoxy-1-(3-methoxy-3-oxopropyl)-4-oxobutyl]-5'-O-(4-methylbenzoyl)adenylyl-(3'.fwdarw.5')-N-(2-methyl-1-oxopropyl)-2'-O-(9-phenyl-9H-xanthen-9-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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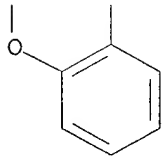
PAGE 2-A



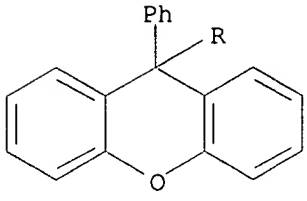
RN 137272-80-1 HCAPLUS
CN Cytidine, N-benzoyl-P-(2-chlorophenyl)-2'-O-[1,4-dimethoxy-1-(3-methoxy-3-oxopropyl)-4-oxobutyl]-5'-O-(4-methylbenzoyl)adenylyl-(3'.fwdarw.5')-N-(2-methyl-1-oxopropyl)-2'-O-(9-phenyl-9H-xanthen-9-yl)guanylyl-(3'.fwdarw.5')-N-benzoyl-, 2',3'-diacetate, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

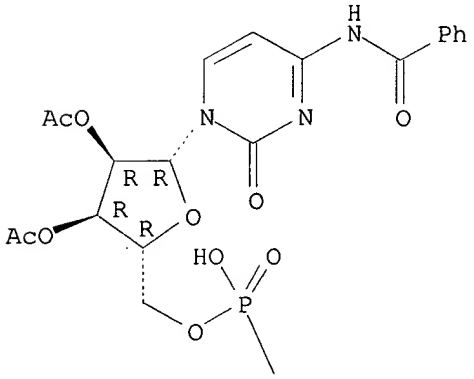
CM 1

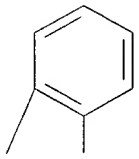
CRN 137272-79-8
CMF C94 H92 Cl N13 O30 P2
CDES 5:B-D-RIBO,B-D-RIBO,B-D-RIBO

Absolute stereochemistry.

PAGE 1-A







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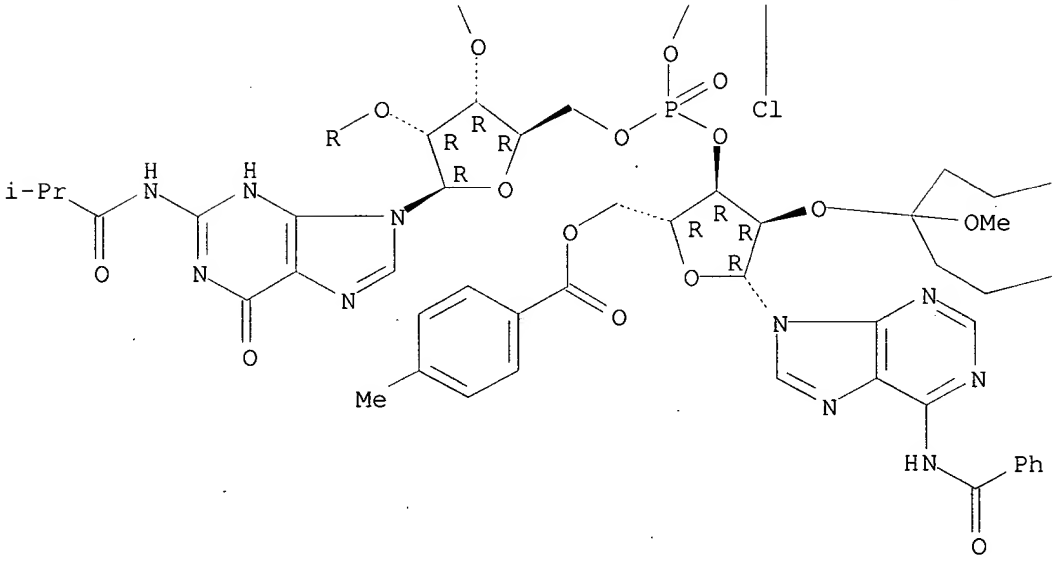
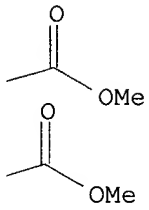
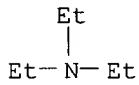




CM 2

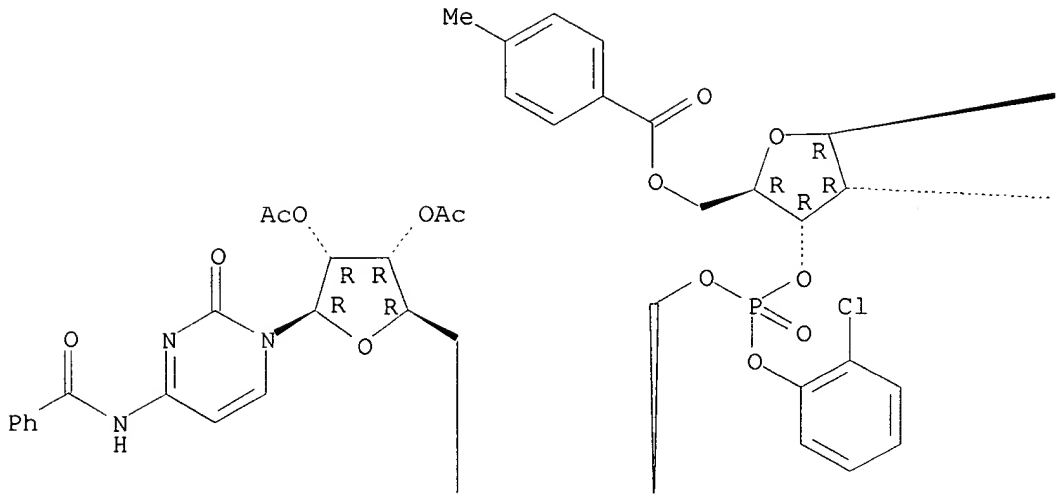
CRN 121-44-8
CMF C6 H15 N



RN 137335-94-5 HCAPLUS
CN Cytidine, N-benzoyl-P-(2-chlorophenyl)-2'-O-[1,4-dimethoxy-1-(3-ethoxy-3-oxopropyl)-4-oxobutyl]-5'-O-(4-methylbenzoyl)adenylyl-(3'.fwdarw.5')-P-(2-chlorophenyl)-N-(2-methyl-1-oxopropyl)-2'-O-(9-phenyl-9H-xanthen-9-yl)guanylyl-(3'.fwdarw.5')-N-benzoyl-, 2',3'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

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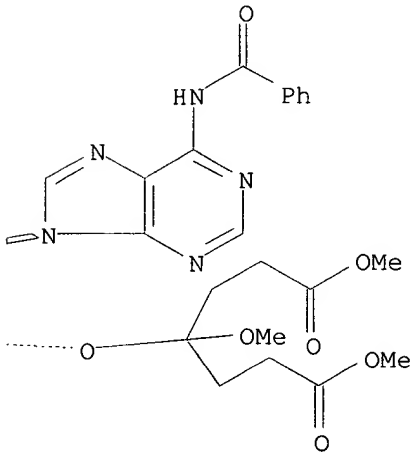

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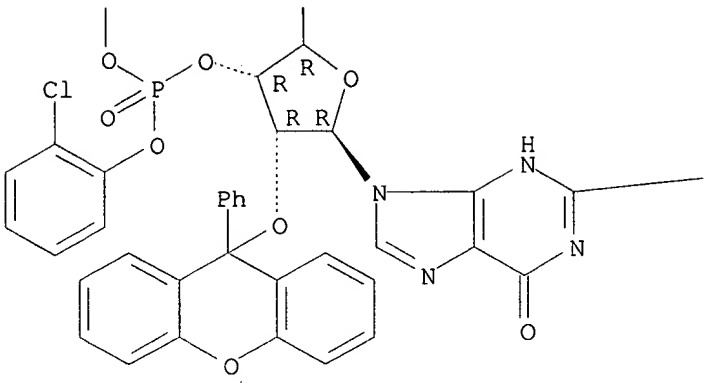
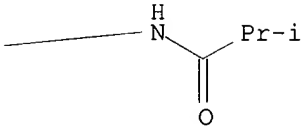


PAGE 2-B



=> d ind 3

L49 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2002 ACS
CC 33-1 (Carbohydrates)
Section cross-reference(s): 22
ST RNA **DNA** conjugate **conformation** NMR;
**oligoribonucleotide** branched prepn **conformation** NMR;
**nucleotide** oligo branched **conformation** NMR
IT **Conformation** and **Conformers**
(of branched **oligoribonucleotides**, NMR in relation to)
IT **Nucleotides**, polymers
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(oligo-, branched RNA-**DNA** conjugate, prepn. and
**conformation** of)
IT 114494-82-5
RL: RCT (Reactant)
(coupling of, with a nucleoside)
IT **137272-75-4**
RL: RCT (Reactant)
(coupling of, with a **nucleotide**)
IT 137272-83-4 137272-84-5
RL: RCT (Reactant)
(coupling of, with **oligoribonucleotides**)
IT 137272-86-7P 137272-87-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and **conformation** of, NMR in relation to)

IT 137272-85-6P 137305-05-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deblocking of)
IT **137272-76-5P** 137272-77-6P **137272-80-1P** 137272-82-3P
**137335-94-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in synthesis of branched
**oligoribonucleotides**)
IT 137272-78-7
RL: RCT (Reactant)
(reaction of, in synthesis of branched **oligoribonucleotides**)

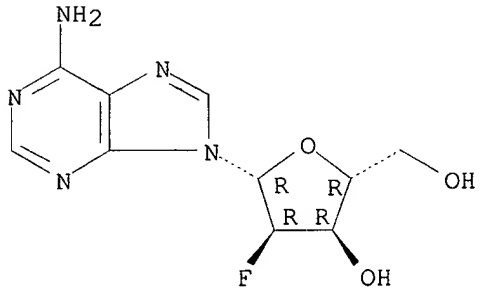
=> d ibib abs hitstr 4

L49 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1982:577180 HCAPLUS
DOCUMENT NUMBER: 97:177180
TITLE: Synthesis and properties of ApU analogs containing 2'-halo-2'-deoxyadenosines. Effects of 2' substituents on **oligonucleotide conformation**
AUTHOR(S): Uesugi, Seiichi; Kaneyasu, Toshinori; Ikehara, Morio
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, 565, Japan
SOURCE: Biochemistry (1982), 21(23), 5870-7
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Five A-U analogs contg. deoxyadensine or 2'-halo-2'-deoxyadenosines, which are known to have widely different C3'-**endo conformer** populations according to their electronegativities of the halogen substituents, d(fluoro)A-U, d(chloro)A-U, d(bromo)A-U, d(iodo)A-U, and dA-U, were synthesized chem. Characterization of these dimers was performed by UV absorption, CD, and1H NMR spectroscopy. The dimers contg. 2'-halo-2'-deoxyadenosines have stacked **conformations** with a **geometry** similar to that of A-U and the degree of stacking decreases in the order d(fluoro)A-U > d(chloro)A-U > d(bromo)A-U > d(iodo)A-U. DeoxychloroA-U is assumed to have the same degree of stacking as A-U. DeoxyA-U takes a more stacked **conformation** than does d(iodo)A-U, but the mode of stacking is different from those of the other dimers. The effects of the 2' substituents on dimer **conformation** are discussed in terms of electronegativity, mol. size, and hydrophobicity.

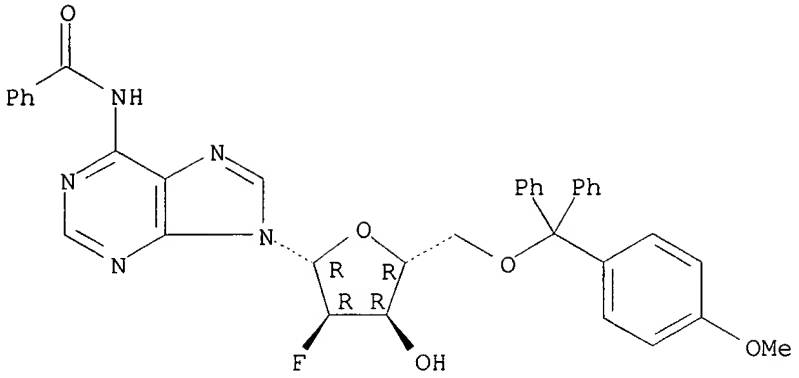
IT **64183-27-3**
RL: BIOL (Biological study)
(monomethoxytritylation of)
RN 64183-27-3 HCAPLUS
CN Adenosine, 2'-deoxy-2'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



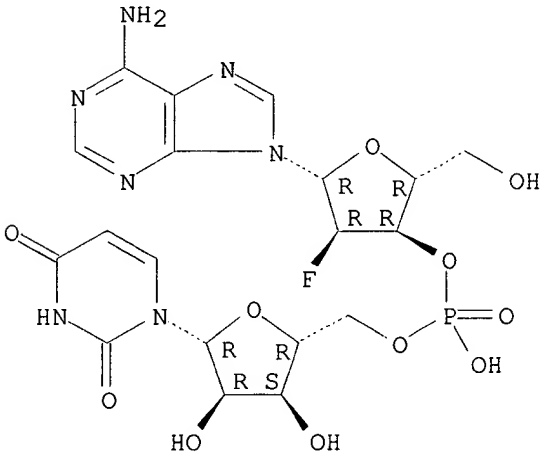

IT **83306-30-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and coupling reaction of, with diacetyl-UMP)
RN 83306-30-3 HCAPLUS
CN Adenosine, N-benzoyl-2'-deoxy-2'-fluoro-5'-O-[(4-methoxyphenyl)diphenylmethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **83306-25-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and properties of)
RN 83306-25-6 HCAPLUS
CN Uridine, 2'-deoxy-2'-fluoroadenylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d ind 4

L49 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2002 ACS
CC 6-2 (General Biochemistry)
ST halodeoxyadenosine uridine **dinucleotide conformation**
IT Circular dichroism
**Conformation** and **Conformers**
Nuclear magnetic resonance
Ultraviolet and visible spectra
(of halo deoxyadenylyl uridines)
IT **Nucleotides**, properties
RL: SPN (Synthetic preparation); PREP (Preparation)
(di-, 2'-halo-, prepn. and properties of)
IT 58-97-9, reactions
RL: RCT (Reactant)

(acetylation of)
IT 48215-95-8
RL: RCT (Reactant)
(coupling reaction of, with halodeoxyadenosine deriv.)
IT 958-09-8 2627-62-5 **64183-27-3** 65446-56-2 68775-04-2
RL: BIOL (Biological study)
(monomethoxytritylation of)
IT **83306-30-3P** 83306-31-4P 83306-32-5P 83306-33-6P
83306-34-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and coupling reaction of, with diacetyl-UMP)
IT **83306-25-6P** 83306-26-7P 83306-27-8P 83306-28-9P
83306-29-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and properties of)
IT 83306-35-8P 83306-36-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectral properties of)

STR Search

KRISHNAN 09/970,971

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=>  d que l64
L13                 STR
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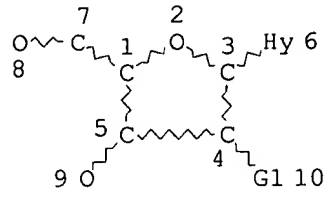

Same STR as for L39

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@20 21 @22      @23 24  25  26

VAR G1=13/23/11/F
REP G2=(1-10) 17-13 18-15
REP G3=(1-10) 20-23 22-25
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT   6
GGCAT   IS LIN  SAT  AT  15
GGCAT   IS LIN  SAT  AT  17
GGCAT   IS LIN  SAT  AT  20
GGCAT.  IS LIN  SAT  AT  25
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M4 C  AT   6
ECOUNT  IS X10 C  AT  15
ECOUNT  IS M2-X10 C  AT  17
ECOUNT  IS M2-X10 C  AT  20
ECOUNT  IS X10 C  AT  25

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  25

STEREO ATTRIBUTES: NONE
L16        5085 SEA FILE=REGISTRY SSS FUL L13
L17         858 SEA FILE=REGISTRY ABB=ON  PLU=ON  L16 AND NCNC3/ES AND
                NCNC2-NCNC3/ES
L18         858 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 AND P/ELS
L19        4227 SEA FILE=REGISTRY ABB=ON  PLU=ON  L16 NOT L18
L20         222 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L18
L21        2311 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19
L61       25301 SEA FILE=HCAPLUS ABB=ON  PLU=ON  A(W)TYPE
L62        7275 SEA FILE=HCAPLUS ABB=ON  PLU=ON  B(W)TYPE
L63        1520 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L61 AND L62
L64           1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L63 AND (L20 OR L21)
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1 citation

=> d ibib abs hitstr

L64 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1982:102141 HCAPLUS
DOCUMENT NUMBER: 96:102141
TITLE: Polynucleotide helix geometry and stability: Spectroscopic, antigenic and interferon-inducing properties of deoxyribose-, ribose- or 2'-deoxy-2'-fluoro-ribose-containing duplexes of poly-inosinic acid.cntdot.poly-cytidylic acid
AUTHOR(S): Kakiuchi, Nobuko; Marck, Christian; Rousseau, Nicole; Leng, Marc; De Clercq, Erik; Guschlbauer, Wilhelm
CORPORATE SOURCE: Dep. Biol., Cent. Etud. Nucl. Saclay, Gif-sur-Yvette, F-91191, Fr.
SOURCE: J. Biol. Chem. (1982), 257(4), 1924-8
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB CD, absorbance temp. profiles, antigenic properties and interferon inducing capacity of 9 double stranded complexes between poly(inosinic acid) and poly(cytidylic acid) [rI)n.cntdot.(rC)n] and their deoxy- and 2'-deoxy-2'-fluoro-analog were studied. The complexes contg. only ribose or 2'-fluororibose chains showed similar CD spectra and thermal stabilities. Anti-(rI)n.cntdot.(rC)n antibodies were well recognized by the duplexes contg. 2'-fluoro-ribose in either strand. These 2 duplexes were also efficient interferon inducers. Presence of fluororibose in both strands decreased the affinity of anti-(rI)n.cntdot.(rC)n antibodies slightly and abolished interferon inducing activity. All polydeoxyriboside contg. complexes showed CD spectra significantly different from the previous group; they showed also 40-100 times lower affinity for the anti-(rI)n.cntdot.(rC)n antibodies, and did not induce interferon. It is concluded that the structure of (rI)n.cntdot.(rC)n, an **A-type** helix, is little perturbed by substitution of one or both strands by 2'-fluororibose. Substitution by deoxyribose in either strand considerably changes the structure of the helices. The hybrids contg. polydeoxycytidylic acid retain at least some of the structural features of the **B-type** helix poly(deoxyinosinic acid).cntdot.poly(deoxycytidylic acid).
IT **63566-69-8 68777-96-8 80145-10-4 80155-11-9 80188-70-1**
RL: BIOL (Biological study)
(interferon induction by, poly I.cntdot.poly C in relation to)
RN 63566-69-8 HCAPLUS
CN 5'-Inosinic acid, homopolymer, complex with 2'-deoxy-2'-fluoro-5'-cytidylic acid homopolymer (1:1) (9CI) (CA INDEX NAME)

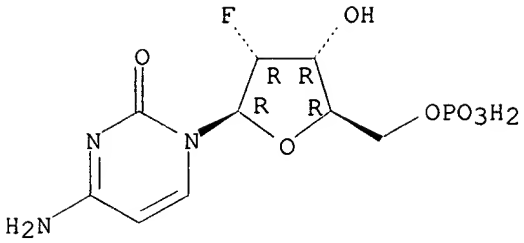
CM 1

CRN 63541-63-9
CMF (C9 H13 F N3 O7 P)x
CCI PMS

CM 2

CRN 63541-62-8
CMF C9 H13 F N3 O7 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



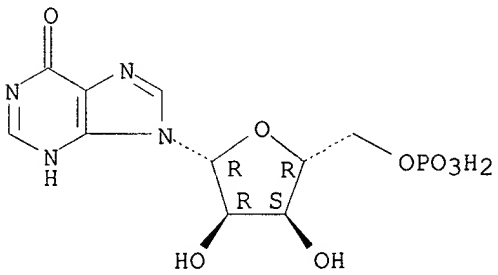
CM 3

CRN 30918-54-8
CMF (C10 H13 N4 O8 P)x
CCI PMS

CM 4

CRN 131-99-7
CMF C10 H13 N4 O8 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



RN 68777-96-8 HCAPLUS
CN 5'-Inosinic acid, 2'-deoxy-2'-fluoro-, homopolymer, complex with 5'-cytidylic acid homopolymer (1:1) (9CI) (CA INDEX NAME)

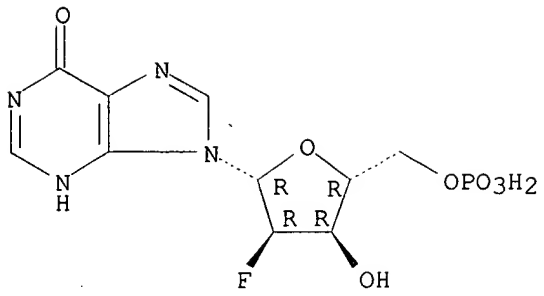
CM 1

CRN 68777-95-7
CMF (C10 H12 F N4 O7 P)x
CCI PMS

CM 2

CRN 68777-94-6
CMF C10 H12 F N4 O7 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



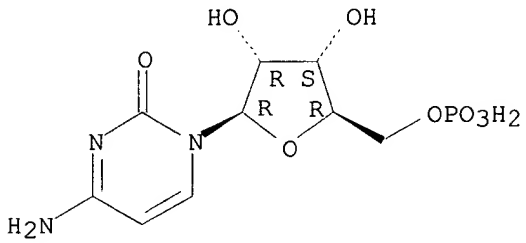
CM 3

CRN 30811-80-4
CMF (C9 H14 N3 O8 P)x
CCI PMS

CM 4

CRN 63-37-6
CMF C9 H14 N3 O8 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



RN 80145-10-4 HCAPLUS
CN 5'-Inosinic acid, 2'-deoxy-2'-fluoro-, homopolymer, complex with 2'-deoxy-5'-cytidylic acid homopolymer (1:1) (9CI) (CA INDEX NAME)

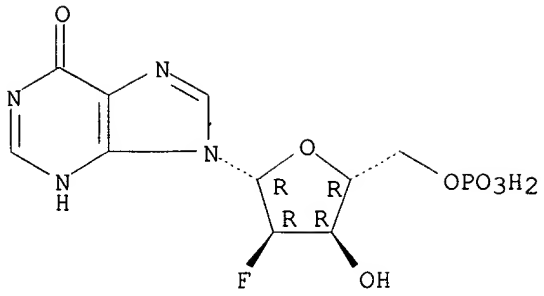
CM 1

CRN 68777-95-7
CMF (C10 H12 F N4 O7 P)x
CCI PMS

CM 2

CRN 68777-94-6
CMF C10 H12 F N4 O7 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



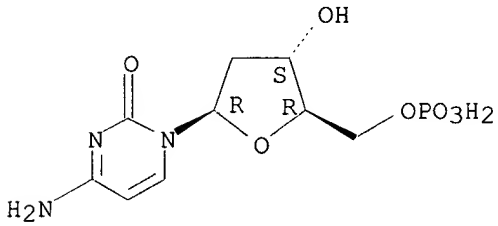
CM 3

CRN 25609-92-1
CMF (C9 H14 N3 O7 P)x
CCI PMS

CM 4

CRN 1032-65-1
CMF C9 H14 N3 O7 P
CDES 5:B-D-ERYTHRO

Absolute stereochemistry.



RN 80155-11-9 HCAPLUS
CN 5'-Inosinic acid, 2'-deoxy-, homopolymer, complex with 2'-deoxy-2'-fluoro-5'-cytidylic acid homopolymer (1:1) (9CI) (CA INDEX NAME)

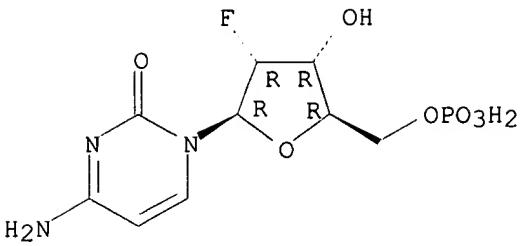
CM 1

CRN 63541-63-9
CMF (C9 H13 F N3 O7 P)x
CCI PMS

CM 2

CRN 63541-62-8
CMF C9 H13 F N3 O7 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



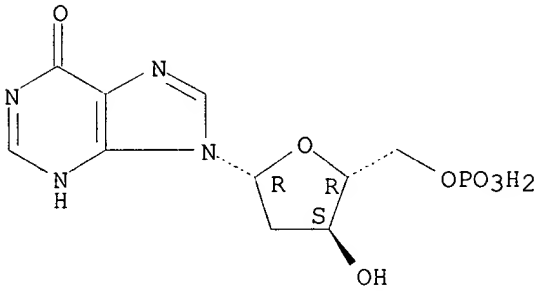
CM 3

CRN 27732-54-3
CMF (C10 H13 N4 O7 P)x
CCI PMS

CM 4

CRN 3393-18-8
CMF C10 H13 N4 O7 P
CDES 5:B-D-ERYTHRO

Absolute stereochemistry.



RN 80188-70-1 HCAPLUS
CN 5'-Inosinic acid, 2'-deoxy-2'-fluoro-, homopolymer, complex with 2'-deoxy-2'-fluoro-5'-cytidylic acid homopolymer (1:1) (9CI) (CA INDEX NAME)

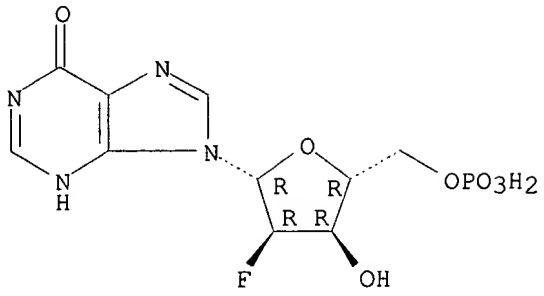
CM 1

CRN 68777-95-7
CMF (C10 H12 F N4 O7 P)x
CCI PMS

CM 2

CRN 68777-94-6
CMF C10 H12 F N4 O7 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



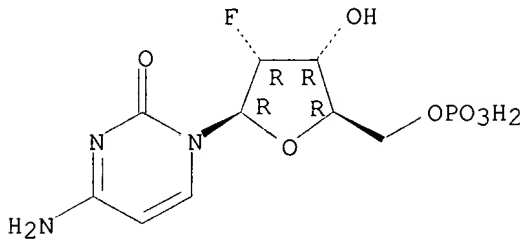
CM 3

CRN 63541-63-9
CMF (C9 H13 F N3 O7 P)x
CCI PMS

CM 4

CRN 63541-62-8
CMF C9 H13 F N3 O7 P
CDES 5:B-D-RIBO

Absolute stereochemistry.



=> d ind

L64 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS
CC 15-2 (Immunochemistry)
Section cross-reference(s): 1
ST polyinosinate polycytidylate analog antigen interferon
IT Interferons
RL: PRP (Properties)
(induction of, by poly I.cntdot.poly C analogs contg. fluororibose)
IT Antibodies
RL: BIOL (Biological study)
(to poly I.cntdot.poly C, fluororibose-contg. analogs recognition by)
IT Molecular structure-biological activity relationship
(interferon-inducing, of poly I.cntdot.poly C analogs contg. fluororibose)
IT 24939-03-5D, fluororibose-contg. analogs
RL: BIOL (Biological study)
(interferon induction by)

IT 24939-03-5 25853-45-6 27380-19-4 **63566-69-8**
**68777-96-8 80145-10-4 80155-11-9**
**80188-70-1**
RL: BIOL (Biological study)
(interferon induction by, poly I.cntdot.poly C in relation to)